Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 06:46 am BST

PDB ID	:	7PWO
EMDB ID	:	EMD-13683
Title	:	Cryo-EM structure of Giardia lamblia ribosome at 2.75 A resolution
Authors	:	Hiregange, D.G.; Rivalta, A.; Bose, T.; Breiner-Goldstein, E.; Samiya, S.; Cimicata, G.; Kulakova, L.; Zimmerman, E.; Bashan, A.; Herzberg, O.; Yonath, A.
Deposited on	:	2021-10-07
Resolution	:	2.75 Å(reported)

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

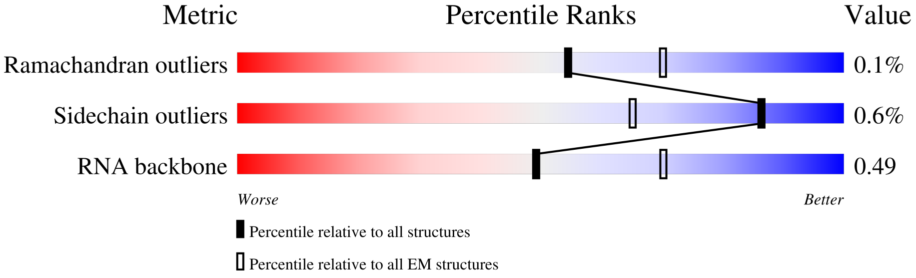
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

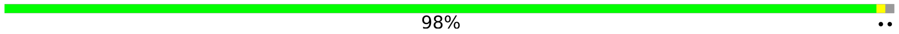
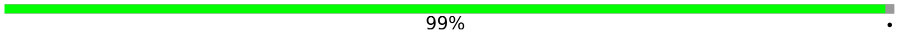
The reported resolution of this entry is 2.75 Å.

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%

Mol	Chain	Length	Quality of chain
1	T1	139	
2	N1	154	
3	J1	189	
4	D1	217	
5	X1	143	
6	S1	154	
7	Q1	158	
8	C1	242	
9	B1	248	

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Mol	Chain	Length	Quality of chain
10	b1	124	63% • 36%
11	a1	109	89% 11%
12	V1	89	92% 8%
13	R1	137	72% • 28%
14	K1	134	62% 38%
15	I1	174	94% 6%
16	e1	69	54% 46%
17	H1	190	85% • 15%
18	n1	41	59% 41%
19	c1	64	84% • 14%
20	O1	145	87% 13%
21	W1	130	99% •
22	E1	268	96% •
23	L1	199	89% • 9%
24	U1	126	59% 41%
25	1	2707	69% 20% • 10%
26	3	120	80% 17% • •
27	42	139	71% 27% ••
28	A2	251	100%
29	B2	379	100%
30	C2	316	99% •
31	D2	297	89% 10%
32	F2	235	91% 9%
33	G2	225	80% 19%
34	H2	185	99% ••

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Mol	Chain	Length	Quality of chain
35	I2	210	95% 5%
36	J2	173	94% • 5%
37	L2	234	81% 19%
38	M2	131	97% ••
39	N2	204	100%
40	O2	197	99% •
41	P2	164	94% 6%
42	Q2	179	99% •
43	R2	196	88% • 10%
44	S2	173	99% •
45	T2	159	96% • •
46	U2	171	58% 42%
47	V2	142	97% ••
48	X2	141	82% 18%
49	Y2	135	99% •
50	Z2	135	96% •
51	a2	149	99% •
52	b2	62	90% 10%
53	c2	109	92% 8%
54	d2	106	89% 11%
55	e2	136	93% 7%
56	f2	123	99% •
57	g2	120	82% 18%
58	h2	124	97% •
59	i2	90	94% 6%

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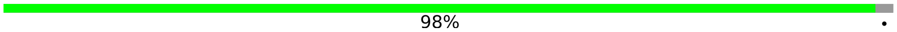
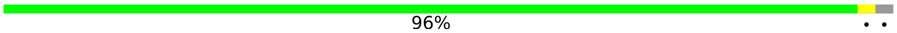
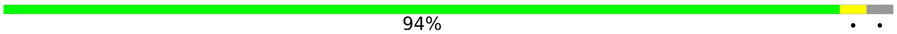
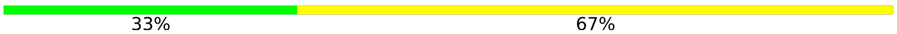
Mol	Chain	Length	Quality of chain
60	j2	89	 98% •
61	k2	77	 86% 14%
62	l2	51	 96% • •
63	m2	127	 39% • 60%
64	o2	106	 89% 11%
65	p2	94	 94% • •
66	w2	14	 29% 57% 14%
67	W2	102	 64% 36%
68	E	3	 33% 67%
69	d1	137	 34% • 65%
70	F1	190	 78% 6% 15%
71	Y1	132	 67% • 31%
72	G1	248	 73% • 24%
73	2	1452	 64% 25% • 7%
74	A1	245	 79% 21%

2 Entry composition ⓘ

There are 76 unique types of molecules in this entry. The entry contains 163704 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 protein called Ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	T1	108	795	503	148	142	2	0	0

- Molecule 2 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	N1	152	1192	759	227	201	5	0	0

- Molecule 3 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J1	166	1322	827	257	232	6	0	0

- Molecule 4 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D1	182	1402	890	254	244	14	0	0

- Molecule 5 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	X1	142	1104	697	219	184	4	0	0

- Molecule 6 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S1	133	1055	651	210	188	6	0	0

- Molecule 7 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Q1	125	960	603	190	164	3	0	0

- Molecule 8 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C1	212	1641	1043	298	296	4	0	0

- Molecule 9 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B1	218	1758	1113	323	309	13	0	0

- Molecule 10 is a protein called Ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	b1	79	614	389	105	114	6	0	0

- Molecule 11 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	a1	97	785	484	162	131	8	0	0

- Molecule 12 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	V1	82	605	377	112	110	6	0	0

- Molecule 13 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	R1	99	767	476	141	147	3	0	0

- Molecule 14 is a protein called Ribosomal protein S10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K1	83	689	446	116	123	4	0	0

- Molecule 15 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	I1	163	1282	804	246	229	3	0	0

- Molecule 16 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	e1	37	291	185	59	46	1	0	0

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	H1	162	1195	773	210	207	5	0	0

- Molecule 18 is a protein called Ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	n1	24	217	134	55	25	3	0	0

- Molecule 19 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	c1	55	439	269	89	80	1	0	0

- Molecule 20 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	O1	126	935	572	189	170	4	0	0

- Molecule 21 is a protein called Ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W1	129	1031	659	192	177	3	0	0

- Molecule 22 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	E1	258	2062	1320	378	352	12	0	0

- Molecule 23 is a protein called SSU ribosomal protein S17P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	L1	181	1487	936	296	248	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L1	12	SER	GLY	conflict	UNP V6TVJ7

- Molecule 24 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	U1	74	609	394	111	102	2	0	0

- Molecule 25 is a RNA chain called rRNA 28S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	1	2448	52571	23373	9743	17007	2448	0	0

- Molecule 26 is a RNA chain called rRNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	3	117	2501	1116	458	810	117	0	0

- Molecule 27 is a RNA chain called rRNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
27	42	138	2958	1315	553	952	138	0	0

- Molecule 28 is a protein called Ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	A2	250	1873	1157	383	320	13	0	0

- Molecule 29 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	B2	378	2987	1886	566	514	21	0	0

- Molecule 30 is a protein called Ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	C2	314	2446	1539	474	424	9	0	0

- Molecule 31 is a protein called Ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	D2	266	2115	1341	391	375	8	0	0

- Molecule 32 is a protein called Ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	F2	214	1730	1100	315	310	5	0	0

- Molecule 33 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	G2	182	1446	921	264	255	6	0	0

- Molecule 34 is a protein called Ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	H2	184	1442	912	263	257	10	0	0

- Molecule 35 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	I2	200	1621	1019	321	273	8	0	0

- Molecule 36 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	J2	164	1305	821	246	233	5	0	0

- Molecule 37 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	L2	189	1512	942	309	255	6	0	0

- Molecule 38 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	M2	128	990	626	178	181	5	0	0

- Molecule 39 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	N2	204	1712	1083	358	265	6	0	0

- Molecule 40 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	O2	195	1587	997	310	267	13	0	0

- Molecule 41 is a protein called Ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	P2	154	Total 1235	C 781	N 239	O 211	S 4	0	0

- Molecule 42 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Q2	178	Total 1402	C 871	N 279	O 243	S 9	0	0

- Molecule 43 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R2	177	Total 1463	C 902	N 313	O 243	S 5	0	0

- Molecule 44 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S2	173	Total 1418	C 895	N 274	O 240	S 9	0	0

- Molecule 45 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T2	153	Total 1226	C 766	N 252	O 201	S 7	0	0

- Molecule 46 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	U2	100	Total 820	C 524	N 141	O 153	S 2	0	0

- Molecule 47 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V2	139	Total 1063	C 668	N 207	O 183	S 5	0	0

- Molecule 48 is a protein called Ribosomal protein L23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	X2	116	936	601	169	163	3	0	0

- Molecule 49 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Y2	133	1076	665	219	184	8	0	0

- Molecule 50 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Z2	129	980	623	179	173	5	0	0

- Molecule 51 is a protein called Ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	a2	148	1201	759	240	199	3	0	0

- Molecule 52 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	b2	56	463	280	104	77	2	0	0

- Molecule 53 is a protein called Ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	c2	100	750	470	132	144	4	0	0

- Molecule 54 is a protein called Ribosomal protein L31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	d2	94	752	482	149	121	0	0

- Molecule 55 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	e2	126	Total	C	N	O	S	0	0
			1039	661	207	165	6		

- Molecule 56 is a protein called Ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	f2	123	Total	C	N	O	S	0	0
			974	619	180	171	4		

- Molecule 57 is a protein called Ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	g2	99	Total	C	N	O	S	0	0
			798	493	167	134	4		

- Molecule 58 is a protein called Ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	h2	120	Total	C	N	O	S	0	0
			960	610	185	160	5		

- Molecule 59 is a protein called Ribosomal protein L36-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	i2	85	Total	C	N	O	S	0	0
			691	438	138	111	4		

- Molecule 60 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	j2	87	Total	C	N	O	S	0	0
			692	423	146	116	7		

- Molecule 61 is a protein called Ribosomal L38e.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	k2	66	Total	C	N	O	S	0	0
			504	320	86	94	4		

- Molecule 62 is a protein called Ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	l2	50	Total	C	N	O	0	0
			434	278	91	65		

- Molecule 63 is a protein called Ubiquitin/Ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	m2	51	Total	C	N	O	S	0	0
			421	257	88	69	7		

- Molecule 64 is a protein called Ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	o2	94	Total	C	N	O	S	0	0
			762	474	157	126	5		

- Molecule 65 is a protein called Ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	p2	91	Total	C	N	O	S	0	0
			708	436	144	122	6		

- Molecule 66 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	w2	14	Total	C	N	O	P	0	0
			299	133	56	96	14		

- Molecule 67 is a protein called Ribosomal protein L24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	W2	65	Total	C	N	O	S	0	0
			540	343	110	85	2		

- Molecule 68 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	E	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 69 is a protein called Ribosomal protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	d1	48	Total 392	C 250	N 72	O 65	S 5	0	0

- Molecule 70 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	F1	161	Total 1246	C 771	N 240	O 227	S 8	0	0

- Molecule 71 is a protein called Ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Y1	91	Total 713	C 454	N 126	O 127	S 6	0	0

- Molecule 72 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	G1	189	Total 1453	C 914	N 280	O 249	S 10	0	0

- Molecule 73 is a RNA chain called rRNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	2	1355	Total 29096	C 12946	N 5388	O 9407	P 1355	0	0

- Molecule 74 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	A1	194	Total 1546	C 998	N 269	O 271	S 8	0	0

- Molecule 75 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
75	N1	3	Total 3	K 3	0
75	X1	1	Total 1	K 1	0
75	S1	2	Total 2	K 2	0

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Mol	Chain	Residues	Atoms	AltConf
75	b1	2	Total K 2 2	0
75	a1	1	Total K 1 1	0
75	I1	2	Total K 2 2	0
75	O1	5	Total K 5 5	0
75	W1	1	Total K 1 1	0
75	E1	4	Total K 4 4	0
75	L1	4	Total K 4 4	0
75	U1	1	Total K 1 1	0
75	1	181	Total K 181 181	0
75	3	1	Total K 1 1	0
75	42	2	Total K 2 2	0
75	A2	4	Total K 4 4	0
75	B2	3	Total K 3 3	0
75	C2	4	Total K 4 4	0
75	I2	1	Total K 1 1	0
75	L2	1	Total K 1 1	0
75	N2	2	Total K 2 2	0
75	V2	1	Total K 1 1	0
75	a2	2	Total K 2 2	0
75	e2	1	Total K 1 1	0
75	j2	1	Total K 1 1	0

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Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
75	o2	1	Total K 1 1	0
75	G1	1	Total K 1 1	0
75	2	222	Total K 222 222	0
75	A1	1	Total K 1 1	0

- Molecule 76 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

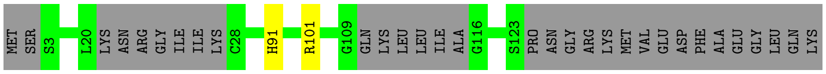
Mol	Chain	Residues	Atoms	AltConf
76	N1	1	Total Mg 1 1	0
76	E1	1	Total Mg 1 1	0
76	L1	1	Total Mg 1 1	0
76	1	71	Total Mg 71 71	0
76	42	1	Total Mg 1 1	0
76	C2	1	Total Mg 1 1	0
76	F2	1	Total Mg 1 1	0
76	P2	1	Total Mg 1 1	0
76	V2	1	Total Mg 1 1	0
76	b2	1	Total Mg 1 1	0
76	o2	1	Total Mg 1 1	0
76	G1	1	Total Mg 1 1	0
76	2	19	Total Mg 19 19	0

3 Residue-property plots ⓘ

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

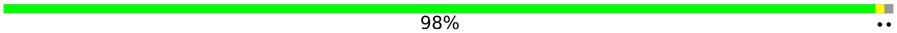
- Molecule 1: Ribosomal protein S19e

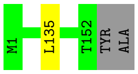
Chain T1:



- Molecule 2: Ribosomal protein S13

Chain N1:



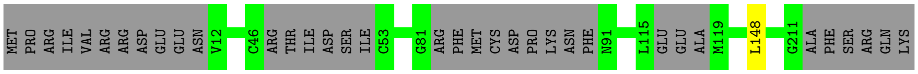


- Molecule 3: Ribosomal protein S9

Chain J1:

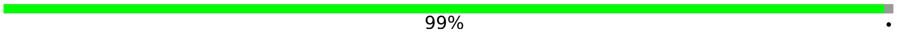
- Molecule 4: Ribosomal protein S3

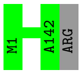
Chain D1:



- Molecule 5: Ribosomal protein S23

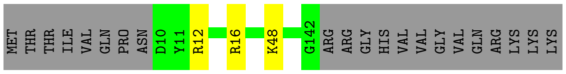
Chain X1:





- Molecule 6: Ribosomal protein S18

Chain S1:

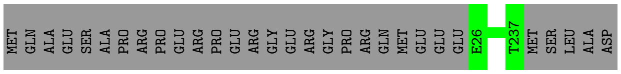


- Molecule 7: Ribosomal protein S16

Chain Q1:

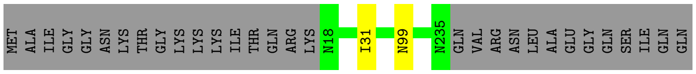
- Molecule 8: Ribosomal protein S2

Chain C1:



- Molecule 9: 40S ribosomal protein S3a

Chain B1:



- Molecule 10: Ribosomal protein S27

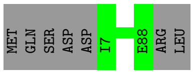
Chain b1:

- Molecule 11: 40S ribosomal protein S26

Chain a1:

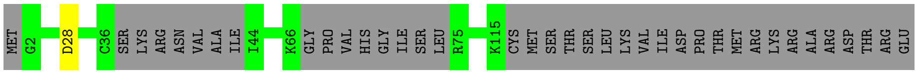
- Molecule 12: 40S ribosomal protein S21

Chain V1:



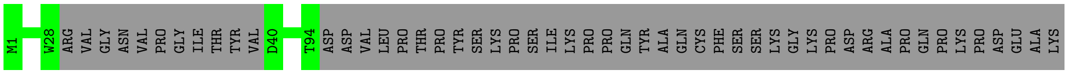
- Molecule 13: Ribosomal protein S17

Chain R1:



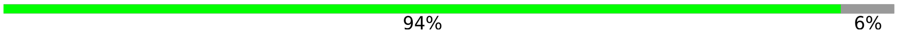
- Molecule 14: Ribosomal protein S10B

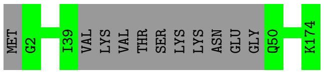
Chain K1:



- Molecule 15: 40S ribosomal protein S8

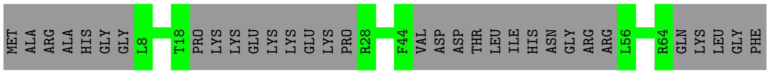
Chain I1:





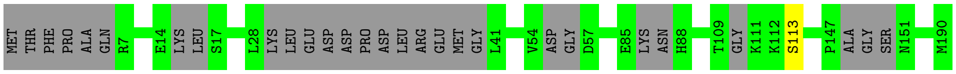
- Molecule 16: 40S ribosomal protein S30

Chain e1:



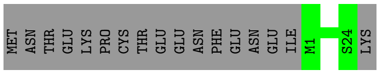
- Molecule 17: 40S ribosomal protein S7

Chain H1:



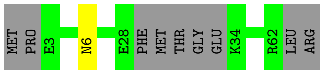
- Molecule 18: Ribosomal protein eL41

Chain n1:



- Molecule 19: Ribosomal protein S28

Chain c1:

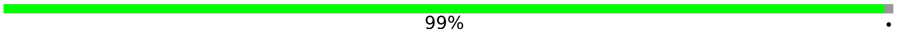


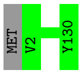
- Molecule 20: Ribosomal protein S14

Chain O1:

- Molecule 21: Ribosomal protein S15A

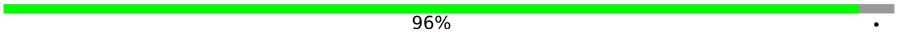
Chain W1:

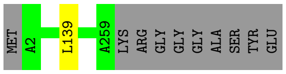




- Molecule 22: 40S ribosomal protein S4

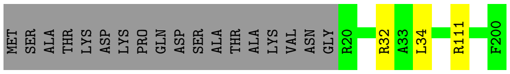
Chain E1:





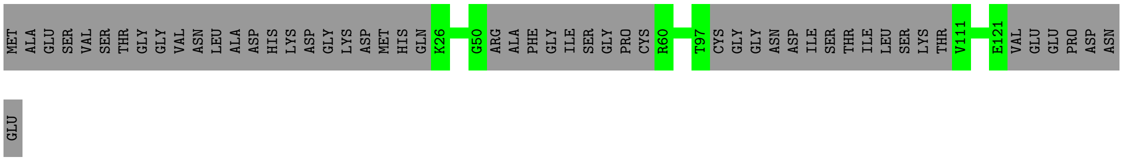
- Molecule 23: SSU ribosomal protein S17P

Chain L1:



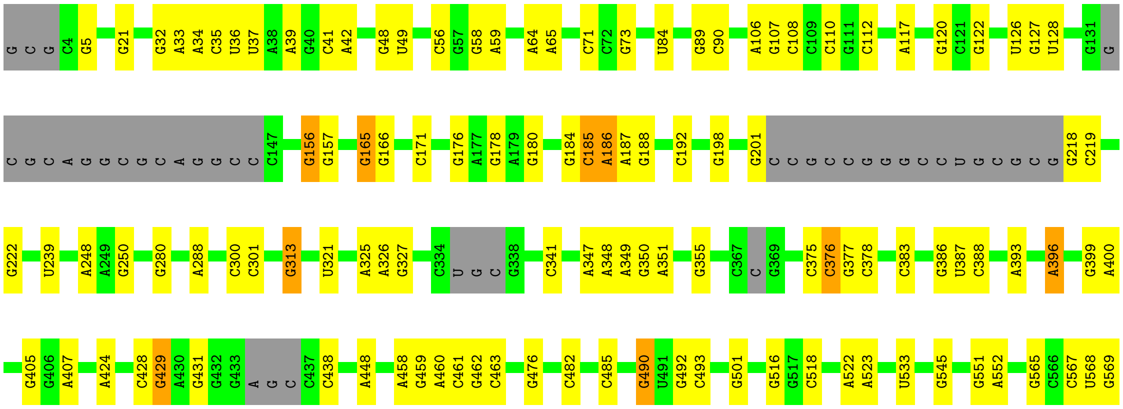
- Molecule 24: Ribosomal protein S20

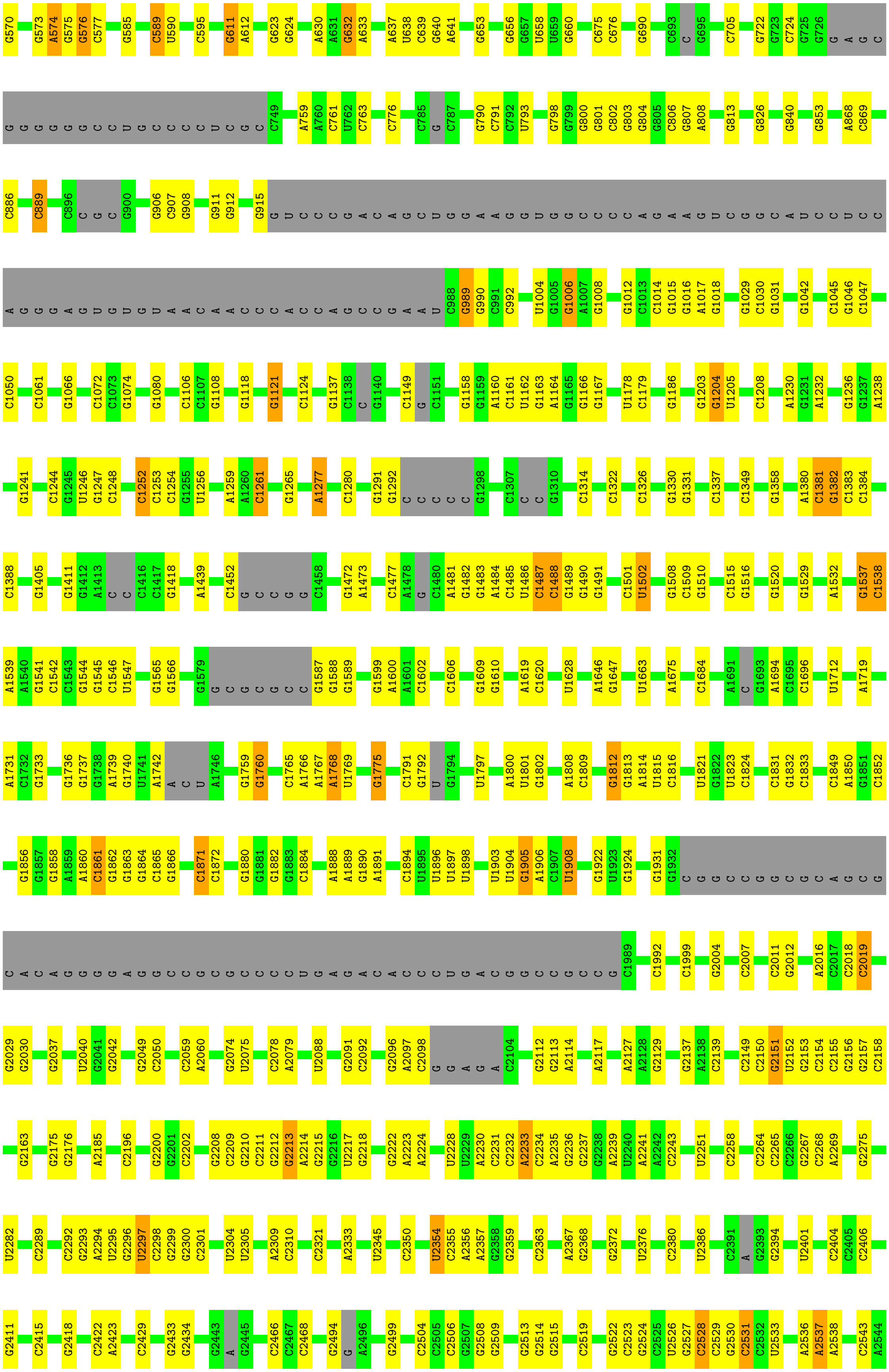
Chain U1:

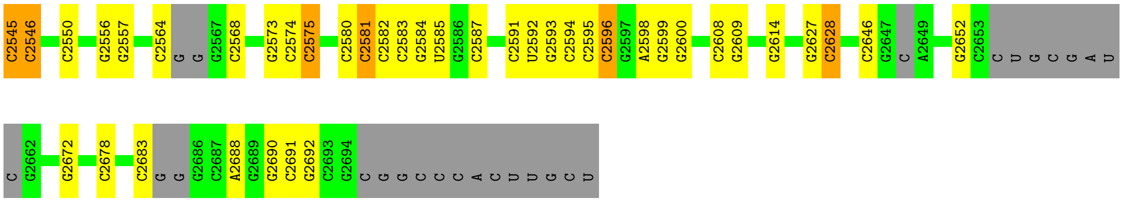


- Molecule 25: rRNA 28S

Chain 1:

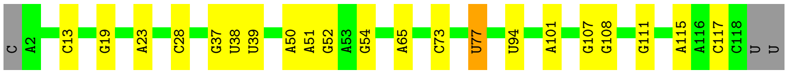



G570 G573 A574 G575 G576 C577 G585 C589 U590 C595 G611 A612 G623 G624 A630 A631 G632 A633 A637 U638 C639 G640 A641 G653 G656 G657 U658 U659 G660 C675 C676 G690 C693 C G695 C705 G722 G723 C724 G725 G726 G A G C
G G G G G G C C U G C C C C U C G C C749 A759 A760 C761 U762 C763 C776 C785 G C787 G790 C791 C792 U793 G798 G799 G800 G801 C802 G803 G804 G805 C806 G807 A808 G813 G826 G840 G853 A868 C869
C886 C889 C896 C G C G900 G906 C907 G908 G911 G912 G915 G U C C C G A C A G C U G G A A G G U G G C C C C A G A A G U C G G C A U C C U C C
A G G G A G U G U G U A A C A A C C C A C C A G C C G A A U C988 G989 G990 C991 C992 U1004 G1005 G1006 A1007 G1008 G1012 C1013 C1014 G1015 G1016 A1017 G1018 G1029 C1030 G1031 G1042 C1045 G1046 C1047
C1050 C1061 G1066 C1072 C1073 G1074 G1080 C1106 C1107 G1108 G1118 G1121 C1124 G1137 C1138 C G1140 C1149 G C1151 G1158 G1159 A1160 C1161 U1162 G1163 A1164 G1165 G1166 G1167 U1178 C1179 G1186 G1203 G1204 U1205 C1208 A1230 G1231 A1232 G1236 G1237 A1238
G1241 C1244 G1245 U1246 G1247 C1248 C1252 C1253 C1254 G1255 U1256 A1259 A1260 C1261 G1265 A1277 C1280 G1291 G1292 C C C C C G1298 C1307 C C G1310 C1314 C1322 C1326 G1330 G1331 C1337 C1349 G1358 A1380 C1381 G1382 C1383 C1384
C1388 G1405 G1411 G1412 A1413 C C C1416 C1417 G1418 A1439 C1452 G C C G G C1458 G1472 A1473 C1477 A1478 G C1480 A1481 G1482 G1483 A1484 C1485 U1486 C1487 C1488 G1489 G1490 G1491 C1501 U1502 G1508 C1509 G1510 C1515 G1516 G1520 G1529 A1532 G1537 C1538
A1539 A1540 G1541 C1542 C1543 G1544 G1545 C1546 U1547 G1565 G1566 G1579 G C G C G C C G1587 G1588 G1589 G1599 A1600 A1601 C1602 C1606 G1609 G1610 A1619 C1620 U1628 A1646 G1647 U1663 A1675 C1684 A1691 C G1693 A1694 C1695 C1696 U1712 A1719
A1731 C1732 G1733 G1736 G1737 G1738 A1739 G1740 U1741 A1742 A C U A1746 G1759 G1760 C1765 A1766 A1767 A1768 U1769 G1775 C1791 G1792 U G1794 U1797 A1800 U1801 G1802 A1808 C1809 G1812 G1813 A1814 U1815 C1816 U1821 G1822 U1823 C1824 C1831 G1832 C1833 C1849 A1850 G1851 C1852
G1856 G1857 G1858 A1859 A1860 C1861 G1862 G1863 G1864 C1865 G1866 C1871 C1872 G1880 G1881 G1882 G1883 C1884 A1888 A1889 G1890 A1891 C1894 U1895 U1896 U1897 U1898 U1903 U1904 G1905 A1906 C1907 U1908 G1922 U1923 G1924 G1931 G1932 C G G C C G G C G C A G C G
C A C A G G G G A G G C C G C G C C C C U G A G A C A C C C U G A C G G C C G C C G C1989 C1992 C1999 G2004 C2007 C2011 G2012 A2016 C2017 C2018 C2019
G2029 G2030 G2037 U2040 G2041 G2042 G2049 C2050 C2059 A2060 G2074 U2075 C2078 A2079 U2088 G2091 C2092 G2096 A2097 C2098 G G A G A C2104 G2112 G2113 A2114 A2117 A2127 A2128 G2129 G2137 A2138 C2139 C2149 C2150 G2151 U2152 G2153 C2154 C2155 G2156 G2157 C2158
G2163 G2175 G2176 A2185 C2196 G2200 G2201 C2202 G2208 C2209 G2210 C2211 G2212 G2213 A2214 G2215 G2216 U2217 G2218 G2222 A2223 A2224 U2228 U2229 A2230 C2231 C2232 A2233 C2234 A2235 G2236 G2237 G2238 A2239 U2240 A2241 A2242 C2243 U2251 C2258 C2264 C2265 C2266 G2267 C2268 A2269 G2275
U2282 C2289 C2292 G2293 A2294 U2295 G2296 U2297 C2298 G2299 G2300 C2301 U2304 U2305 A2309 C2310 C2321 A2333 U2345 C2350 U2354 C2355 A2356 A2357 G2358 G2359 C2363 A2367 G2368 G2372 U2376 C2380 U2386 C2391 A G2393 G2394 U2401 C2404 C2405 C2406
G2411 C2415 G2418 C2422 A2423 C2429 G2433 G2434 G2443 A G2445 C2466 C2467 C2468 G2494 G A2496 G2499 C2504 C2505 C2506 G2507 G2508 G2509 G2513 G2514 G2515 C2519 G2522 C2523 G2524 C2525 U2526 G2527 C2528 C2529 G2530 C2531 C2532 U2533 A2536 A2537 A2538 C2543 A2544



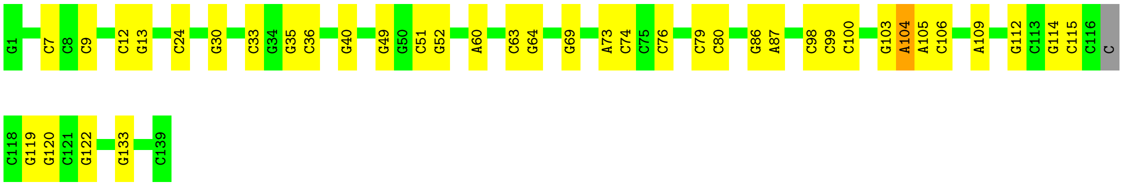
- Molecule 26: rRNA 5S

Chain 3:



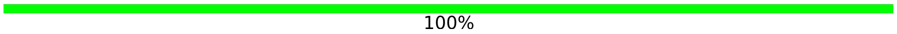
- Molecule 27: rRNA 5.8S

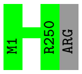
Chain 42:



- Molecule 28: Ribosomal protein L2

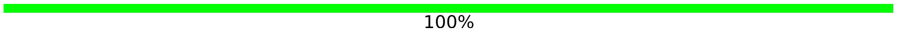
Chain A2:

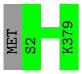




- Molecule 29: Ribosomal protein L3

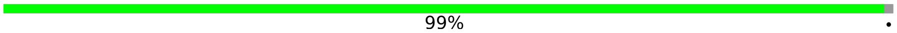
Chain B2:

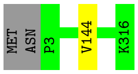




- Molecule 30: Ribosomal protein L4

Chain C2:



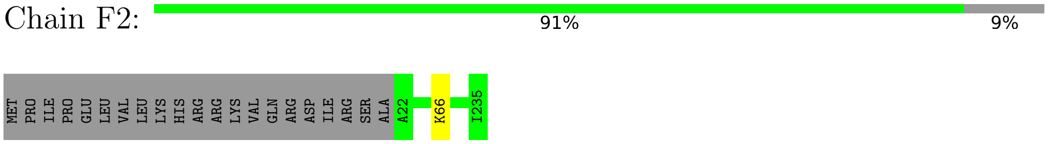


- Molecule 31: Ribosomal protein L5

Chain D2:

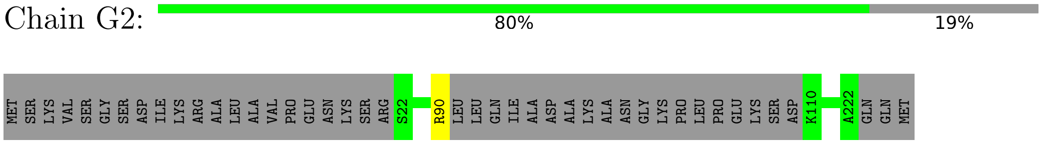
- Molecule 32: Ribosomal protein L7

Chain F2:



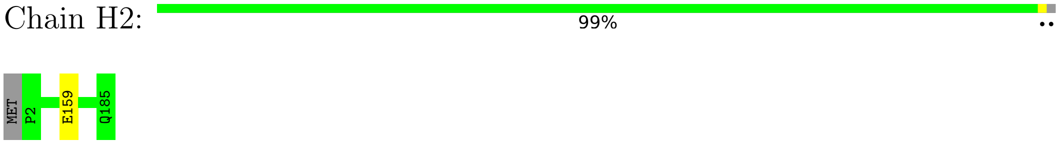
- Molecule 33: 60S ribosomal protein L7a

Chain G2:



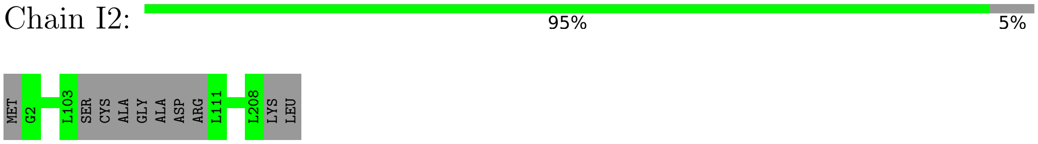
- Molecule 34: Ribosomal protein L6

Chain H2:



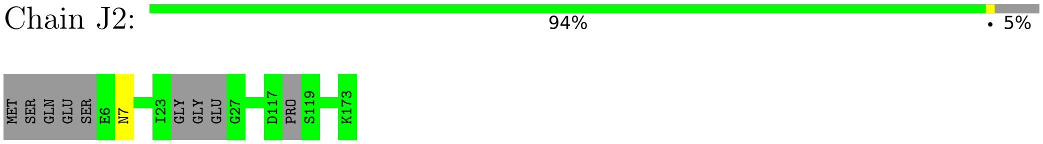
- Molecule 35: Ribosomal protein L10

Chain I2:



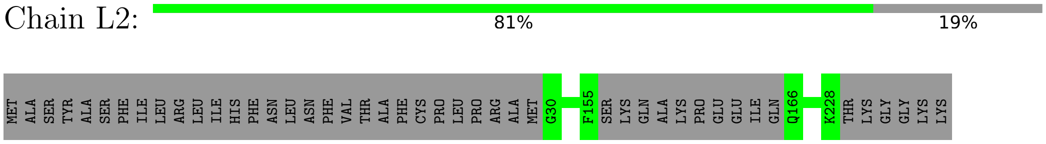
- Molecule 36: Ribosomal protein L11

Chain J2:



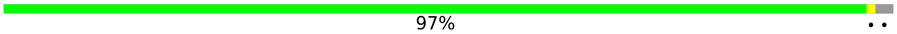
- Molecule 37: 60S ribosomal protein L13

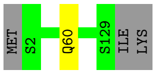
Chain L2:



- Molecule 38: Ribosomal protein L14

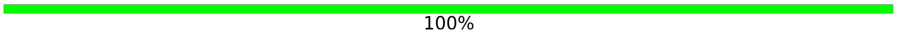
Chain M2:

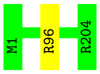




- Molecule 39: Ribosomal protein L15

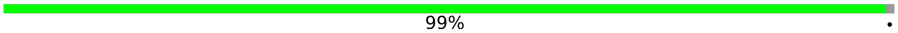
Chain N2:

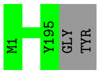




- Molecule 40: Ribosomal protein L13a

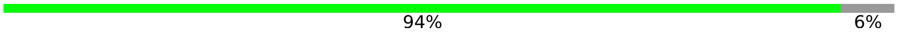
Chain O2:

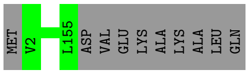




- Molecule 41: Ribosomal protein L17

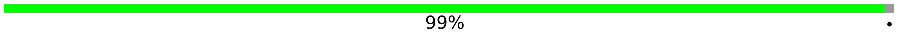
Chain P2:

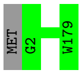




- Molecule 42: Ribosomal protein L18

Chain Q2:



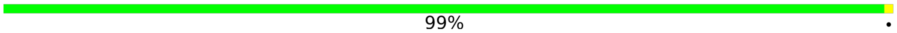


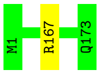
- Molecule 43: Ribosomal protein L19

Chain R2:

- Molecule 44: 60S ribosomal protein L18a

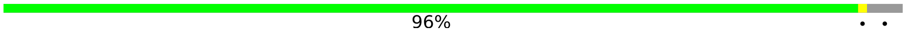
Chain S2:





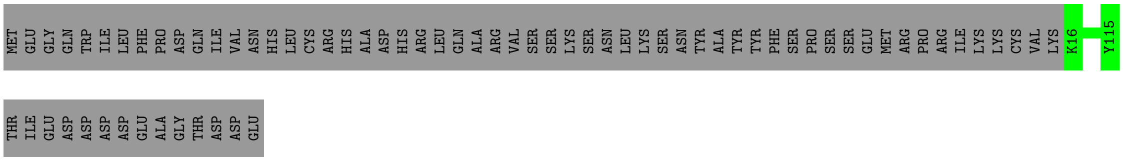
- Molecule 45: Ribosomal protein L21

Chain T2:

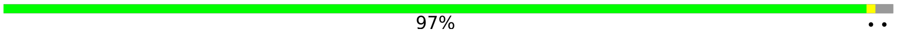


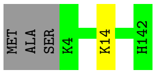
- Molecule 46: Ribosomal protein eL22

Chain U2:

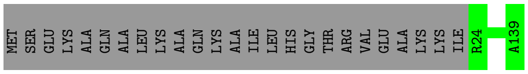
- Molecule 47: Ribosomal protein L23

Chain V2:


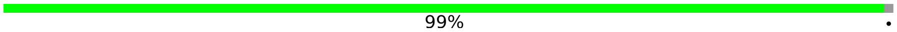


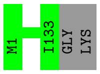
- Molecule 48: Ribosomal protein L23A

Chain X2:

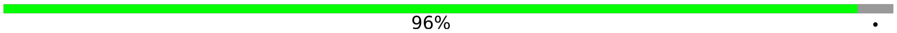



- Molecule 49: Ribosomal protein L26

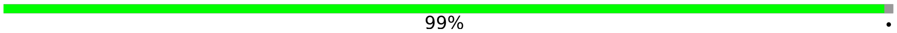
Chain Y2:


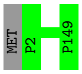


- Molecule 50: 60S ribosomal protein L27

Chain Z2:


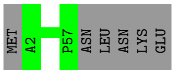
- Molecule 51: Ribosomal protein L27a

Chain a2:




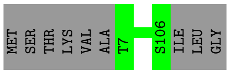
- Molecule 52: 60S ribosomal protein L29

Chain b2:



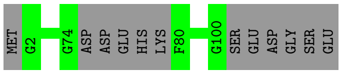
- Molecule 53: Ribosomal protein L30

Chain c2:



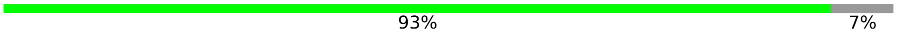
- Molecule 54: Ribosomal protein L31B

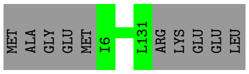
Chain d2:



- Molecule 55: Ribosomal protein L32

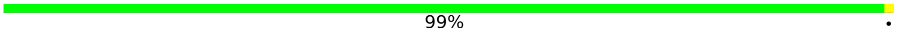
Chain e2:

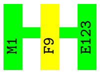




- Molecule 56: Ribosomal protein L35a

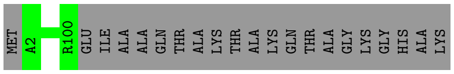
Chain f2:





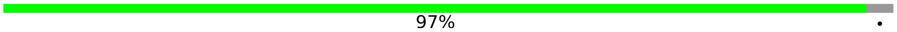
- Molecule 57: Ribosomal protein L34

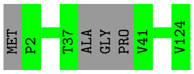
Chain g2:



- Molecule 58: Ribosomal protein L35

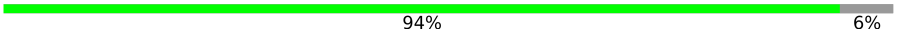
Chain h2:

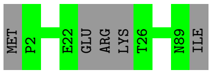




- Molecule 59: Ribosomal protein L36-1

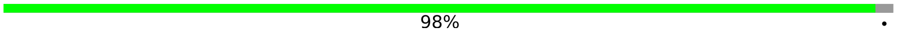
Chain i2:

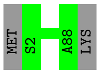




- Molecule 60: Ribosomal protein L37

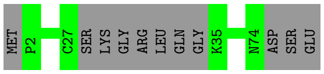
Chain j2:





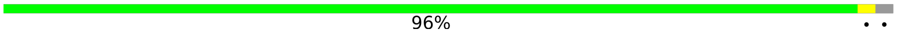
- Molecule 61: Ribosomal L38e

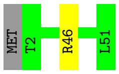
Chain k2:



- Molecule 62: Ribosomal protein L39

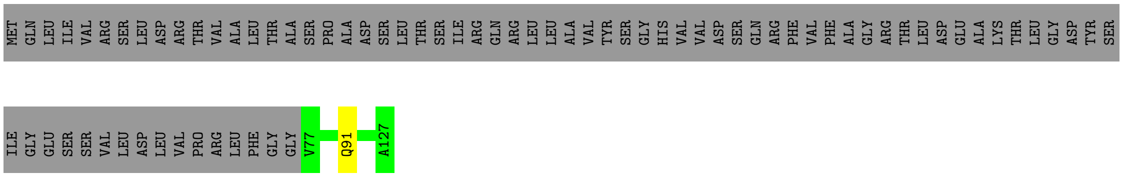
Chain l2:





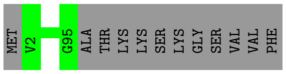
- Molecule 63: Ubiquitin/Ribosomal protein L40e

Chain m2:



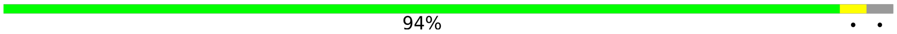
- Molecule 64: Ribosomal protein L44

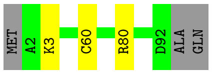
Chain o2:



- Molecule 65: Ribosomal protein L37a

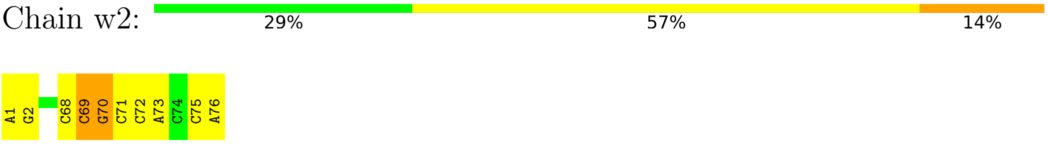
Chain p2:





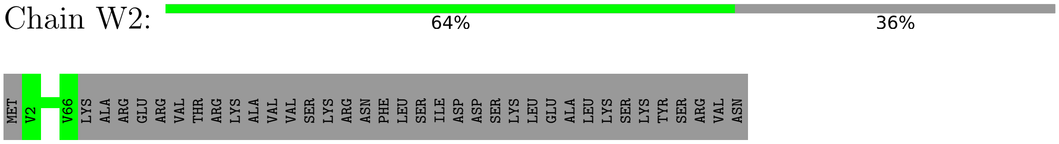
- Molecule 66: E-site tRNA

Chain w2:



- Molecule 67: Ribosomal protein L24A

Chain W2:

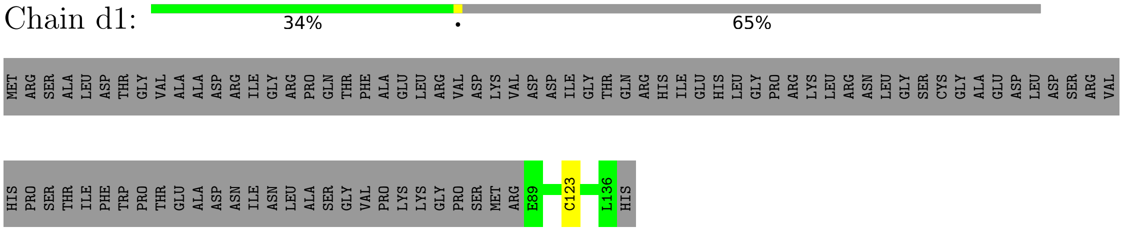


- Molecule 68: P-site tRNA

Chain E:

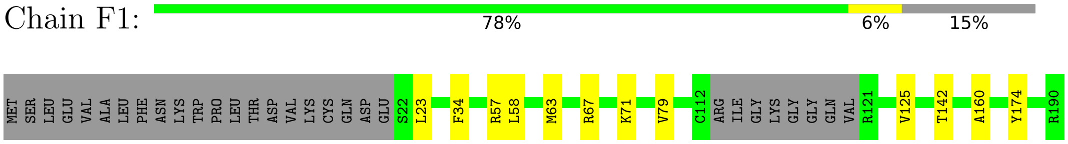
- Molecule 69: Ribosomal protein S29A

Chain d1:



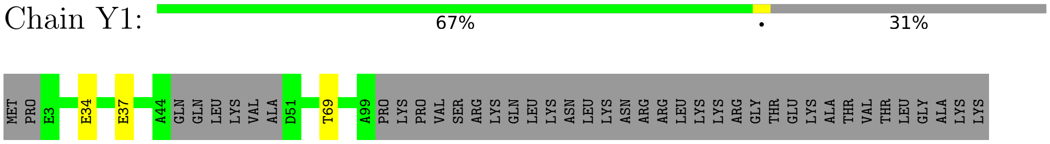
- Molecule 70: Ribosomal protein S5

Chain F1:



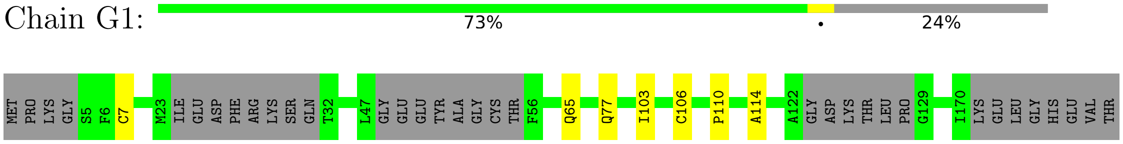
- Molecule 71: Ribosomal protein S24

Chain Y1:



- Molecule 72: 40S ribosomal protein S6

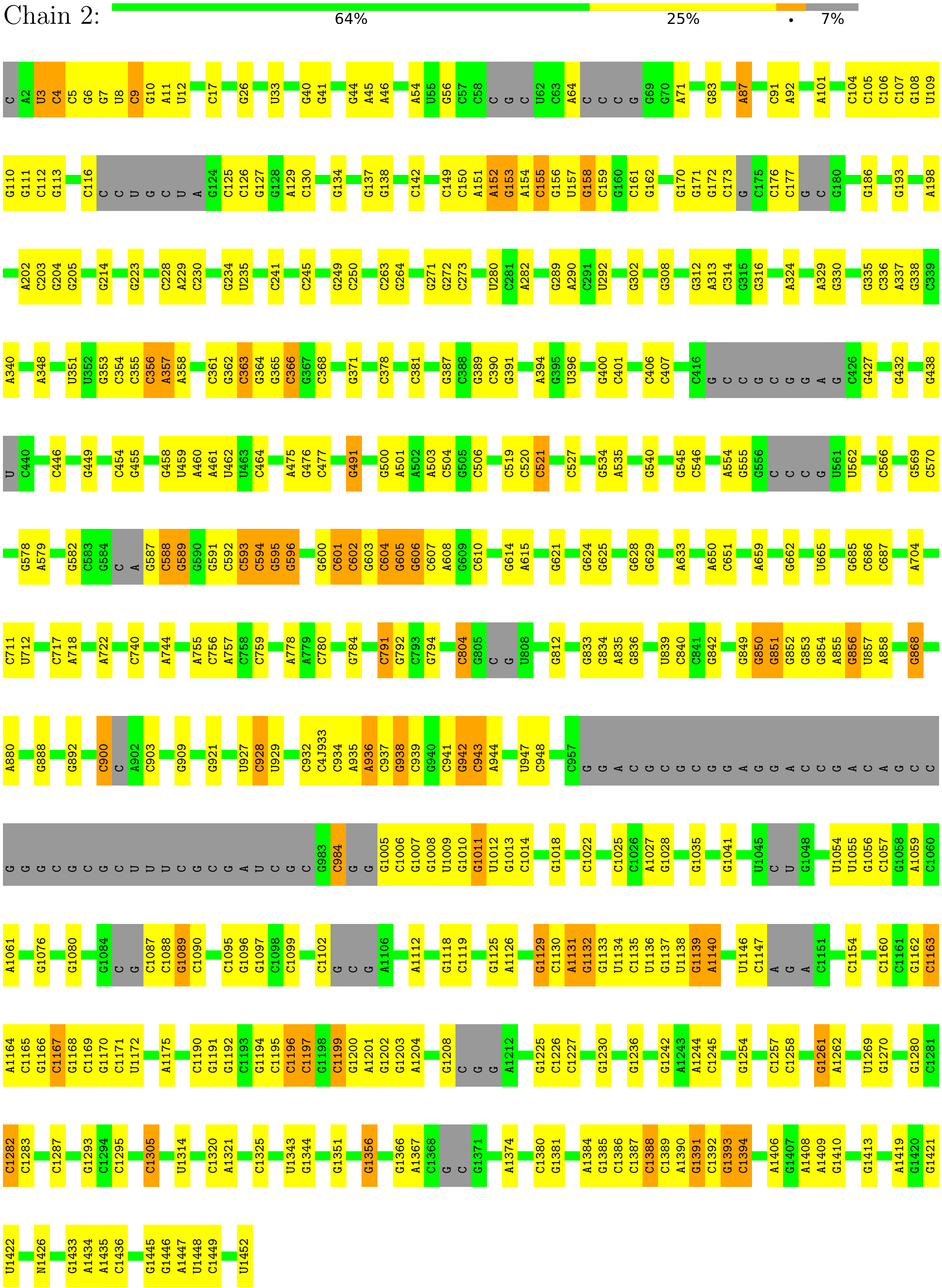
Chain G1:



LEU LYS ASN GLY GLU LYS LYS L186 K187 TYR P189 M231 GLY LYS GLN HIS ASN ILE ARG ILE TYR LYS PRO ALA LYS ARG THR VAL GLU

- Molecule 73: rRNA 18S

Chain 2:



C A2 U3 C4 C5 G6 G7 U8 C9 G10 A11 U12 C17 G26 U33 G40 G41 G44 A45 A46 A54 U55 G56 C57 C58 C G C U62 C63 A64 C C C G G69 G70 A71 G83 A87 C91 A92 A101 C104 C105 C106 C107 G108 U109

G110 G111 C112 G113 C116 C C U G C U A G124 C125 C126 G127 G128 A129 C130 G134 G137 G138 C142 C149 C150 A151 A152 G153 A154 C155 G156 U157 G158 C159 G160 C161 G162 G170 G171 G172 C173 G C175 C176 C177 G C G180 G186 G193 A198

A202 C203 G204 G205 G214 G223 C228 A229 C230 G234 U235 C241 C245 G249 C250 C263 G264 G271 G272 C273 U280 C281 A282 G289 A290 C291 U292 G302 G308 G312 A313 C314 G315 U316 A324 A329 G330 G335 C336 A337 G338 C339

A340 A348 U351 U352 G353 C354 C355 C356 A357 A358 C361 G362 C363 G364 G365 C366 G367 C368 G371 C378 C381 G387 C388 G389 C390 G391 A394 G395 U396 G400 C401 C406 C407 C416 G C C C G G G A G C426 G427 G432 G438

U C440 C446 G449 C454 G455 G458 U459 A460 A461 U462 U463 C464 A475 G476 C477 G491 G500 A501 A502 A503 C504 G505 C506 C519 C520 C521 C527 G534 A535 G540 G545 C546 A554 G555 G556 C C C G U561 U562 C566 G569 C570

G578 A579 G582 C583 G584 C A G587 C588 G589 G590 C591 C592 C593 C594 G595 G596 G600 C601 C602 G603 C604 G605 G606 C607 A608 G609 C610 G614 A615 G621 G624 G625 G628 G629 A633 A650 C651 A659 G662 U665 G685 C686 C687 A704

C711 U712 C717 A718 A722 C740 A744 A755 C756 A757 C758 C759 A778 A779 C780 G784 C791 G792 C793 G794 C804 G805 C G U808 G812 G833 G834 A835 G836 U839 C840 C841 G842 G849 G850 G851 G852 G853 G854 A855 G856 U857 A858 G868

A880 G888 G892 C900 C A902 C903 G909 G921 U927 C928 U929 C932 C4J933 C934 A935 A936 C937 G938 C939 G940 C941 G942 C943 A944 U947 C948 C957 G G A C G C G C G G A G G A C C G A C A G C C

G G G C G C G C U U U C G C G A U C G C G983 C984 G G G1005 C1006 G1007 G1008 U1009 G1010 G1011 U1012 G1013 C1014 G1018 C1022 C1025 C1026 A1027 G1028 G1035 G1041 U1045 C U G1048 U1054 U1055 G1056 C1057 G1058 A1059 C1060

A1061 G1076 G1080 G1084 C G C1087 C1088 G1089 C1090 C1095 G1096 G1097 C1098 C1099 C1102 G C G A1106 A1112 G1118 C1119 G1125 A1126 G1129 C1130 A1131 G1132 G1133 U1134 C1135 U1136 G1137 U1138 G1139 A1140 U1146 C1147 A G A C1151 C1154 C1160 C1161 G1162 C1163

A1164 C1165 G1166 C1167 G1168 C1169 G1170 C1171 U1172 A1175 C1190 G1191 G1192 C1193 G1194 C1195 C1196 C1197 G1198 C1199 G1200 A1201 G1202 G1203 A1204 G1208 C G G A1212 G1225 C1226 C1227 G1230 G1236 G1242 A1243 A1244 C1245 G1254 C1257 C1258 G1261 A1262 U1269 G1270 G1280 C1281

C1282 C1283 C1287 G1293 C1294 C1295 C1305 U1314 C1320 A1321 C1325 U1343 G1344 G1351 G1356 G1366 A1367 C1368 G C G1371 A1374 C1380 G1381 A1384 G1385 C1386 C1387 C1388 C1389 A1390 G1391 C1392 G1393 C1394 A1406 G1407 A1408 A1409 G1410 G1413 A1419 G1420 G1421

U1422 N1426 G1433 A1434 A1435 C1436 G1445 G1446 A1447 U1448 C1449 U1452

- Molecule 74: 40S ribosomal protein SA

Chain A1:


79%
21%


MET
SER
THR
GLU
LYS
THR
SER
GLN
ALA
SER
LYS
GLU
TYR
GLN
LEU
LYS
E17
R38
L210
PRO
GLU
GLU
ILE
PRO
ASP
GLU
GLU
GLU
SER
GLU
ASP
PHE
TYR
ASP
ASP
ASP
GLU
GLU
GLU
ASP
GLU
GLU
PHE
SER
ALA
GLY
ASN
GLY
ASN
LEU
PHE
ASP
GLU
TYR

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M7A, 4AC, 7MG, OMU, C4J, OMC, MG, K, OMG, 5MC, MA6, A2M, 4OC

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	T1	0.33	0/812	0.56	0/1098
2	N1	0.35	0/1215	0.59	1/1634 (0.1%)
3	J1	0.34	0/1340	0.63	0/1796
4	D1	0.37	0/1422	0.60	1/1909 (0.1%)
5	X1	0.34	0/1119	0.63	0/1498
6	S1	0.33	0/1070	0.68	0/1435
7	Q1	0.35	0/968	0.64	0/1295
8	C1	0.36	0/1674	0.59	0/2259
9	B1	0.36	0/1793	0.61	1/2419 (0.0%)
10	b1	0.38	0/628	0.78	1/852 (0.1%)
11	a1	0.34	0/797	0.54	0/1072
12	V1	0.41	0/613	0.61	0/823
13	R1	0.38	0/773	0.61	0/1037
14	K1	0.34	0/707	0.64	0/957
15	I1	0.33	0/1302	0.59	0/1746
16	e1	0.31	0/294	0.53	0/392
17	H1	0.34	0/1211	0.55	0/1640
18	n1	0.36	0/219	0.64	0/280
19	c1	0.47	0/439	0.63	0/585
20	O1	0.34	0/947	0.59	0/1273
21	W1	0.37	0/1048	0.59	0/1412
22	E1	0.33	0/2108	0.60	1/2845 (0.0%)
23	L1	0.35	0/1520	0.63	1/2037 (0.0%)
24	U1	0.35	0/619	0.64	0/833
25	1	0.78	0/58145	1.10	239/90686 (0.3%)
26	3	0.61	0/2797	1.00	7/4359 (0.2%)
27	42	0.75	0/3277	1.03	4/5109 (0.1%)
28	A2	0.39	0/1906	0.63	0/2561
29	B2	0.38	0/3058	0.59	0/4129
30	C2	0.40	0/2498	0.61	0/3388
31	D2	0.35	0/2157	0.56	0/2899
32	F2	0.39	0/1760	0.59	0/2374

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	G2	0.37	0/1472	0.59	0/1989
34	H2	0.37	0/1469	0.61	1/1985 (0.1%)
35	I2	0.36	0/1657	0.61	0/2219
36	J2	0.35	0/1325	0.59	0/1776
37	L2	0.38	0/1533	0.59	0/2052
38	M2	0.36	0/1002	0.59	0/1349
39	N2	0.40	0/1755	0.62	0/2353
40	O2	0.41	0/1618	0.58	0/2169
41	P2	0.40	0/1261	0.63	0/1688
42	Q2	0.34	0/1425	0.59	0/1907
43	R2	0.60	0/1478	0.64	0/1954
44	S2	0.38	0/1452	0.57	0/1955
45	T2	0.37	0/1251	0.59	1/1682 (0.1%)
46	U2	0.41	0/836	0.59	0/1124
47	V2	0.35	0/1083	0.58	0/1458
48	X2	0.35	0/956	0.60	0/1293
49	Y2	0.36	0/1091	0.61	0/1454
50	Z2	0.37	0/997	0.54	0/1352
51	a2	0.40	0/1231	0.60	0/1647
52	b2	0.34	0/471	0.56	0/624
53	c2	0.33	0/758	0.64	0/1025
54	d2	0.36	0/764	0.62	0/1026
55	e2	0.39	0/1063	0.56	0/1418
56	f2	0.37	0/994	0.61	1/1338 (0.1%)
57	g2	0.34	0/813	0.54	0/1092
58	h2	0.36	0/971	0.61	0/1295
59	i2	0.36	0/700	0.55	0/927
60	j2	0.38	0/708	0.59	0/941
61	k2	0.33	0/507	0.57	0/679
62	l2	0.34	0/445	0.64	0/594
63	m2	0.34	0/426	0.56	0/568
64	o2	0.40	0/773	0.62	0/1023
65	p2	0.39	0/717	0.71	1/956 (0.1%)
66	w2	0.93	1/332 (0.3%)	1.40	7/511 (1.4%)
67	W2	0.37	0/551	0.58	0/738
68	E	0.43	0/68	1.11	1/103 (1.0%)
69	d1	0.45	0/400	0.60	0/532
70	F1	0.65	0/1264	0.63	0/1697
71	Y1	0.45	0/724	0.67	0/971
72	G1	0.42	0/1466	0.67	0/1956
73	2	0.62	0/32117	1.10	172/50066 (0.3%)
74	A1	0.31	0/1580	0.50	0/2149
All	All	0.60	1/173740 (0.0%)	0.93	440/254267 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	w2	1	A	OP3-P	-10.48	1.48	1.61

All (440) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	2	155	C	P-O3'-C3'	-10.72	106.83	119.70
73	2	595	G	P-O3'-C3'	-10.62	106.96	119.70
73	2	138	G	P-O3'-C3'	-10.38	107.24	119.70
73	2	606	G	P-O3'-C3'	-10.24	107.41	119.70
10	b1	96	PHE	C-N-CA	10.16	147.09	121.70
26	3	52	G	P-O3'-C3'	-10.05	107.64	119.70
73	2	937	C	P-O3'-C3'	-9.90	107.82	119.70
73	2	1007	G	P-O3'-C3'	-9.88	107.85	119.70
25	1	2376	U	P-O3'-C3'	-9.80	107.94	119.70
73	2	366	C	P-O3'-C3'	-9.71	108.05	119.70
73	2	156	G	P-O3'-C3'	-9.70	108.07	119.70
73	2	1132	G	P-O3'-C3'	-9.64	108.13	119.70
25	1	2156	G	P-O3'-C3'	-9.56	108.22	119.70
73	2	9	C	P-O3'-C3'	-9.53	108.27	119.70
73	2	111	G	P-O3'-C3'	-9.51	108.29	119.70
73	2	1135	C	P-O3'-C3'	-9.41	108.41	119.70
73	2	1133	G	P-O3'-C3'	-9.38	108.44	119.70
73	2	943	C	P-O3'-C3'	-9.35	108.48	119.70
73	2	109	U	P-O3'-C3'	-9.28	108.56	119.70
73	2	1011	OMG	P-O3'-C3'	-9.27	108.58	119.70
25	1	1547	U	P-O3'-C3'	-9.25	108.60	119.70
73	2	127	G	P-O3'-C3'	-9.21	108.64	119.70
25	1	1326	C	P-O3'-C3'	-9.20	108.67	119.70
73	2	594	C	P-O3'-C3'	-9.19	108.67	119.70
73	2	1137	G	P-O3'-C3'	-9.17	108.70	119.70
73	2	939	C	P-O3'-C3'	-9.15	108.72	119.70
73	2	1168	G	P-O3'-C3'	-9.12	108.76	119.70
73	2	1392	C	P-O3'-C3'	-9.01	108.88	119.70
25	1	1849	C	C6-N1-C2	-9.00	116.70	120.30
25	1	386	OMG	P-O3'-C3'	-8.88	109.05	119.70
25	1	1833	C	P-O3'-C3'	-8.88	109.05	119.70
25	1	2537	A	P-O3'-C3'	-8.74	109.21	119.70
73	2	11	A	P-O3'-C3'	-8.74	109.21	119.70
73	2	4	C	P-O3'-C3'	-8.72	109.23	119.70
25	1	889	C	C2-N1-C1'	-8.72	109.21	118.80
73	2	363	C	P-O3'-C3'	-8.72	109.24	119.70
73	2	1172	U	P-O3'-C3'	-8.62	109.35	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	1487	C	P-O3'-C3'	-8.59	109.40	119.70
73	2	6	G	P-O3'-C3'	-8.56	109.43	119.70
73	2	521	C	C2-N1-C1'	8.56	128.22	118.80
25	1	355	G	O4'-C1'-N9	8.54	115.03	108.20
73	2	159	C	P-O3'-C3'	-8.53	109.46	119.70
25	1	2154	C	P-O3'-C3'	-8.51	109.48	119.70
73	2	361	C	P-O3'-C3'	-8.51	109.49	119.70
73	2	1138	U	P-O3'-C3'	-8.49	109.50	119.70
73	2	5	C	P-O3'-C3'	-8.49	109.51	119.70
73	2	1008	G	P-O3'-C3'	-8.44	109.57	119.70
73	2	12	U	P-O3'-C3'	-8.43	109.59	119.70
73	2	1140	A	P-O3'-C3'	-8.43	109.59	119.70
73	2	1131	A	P-O3'-C3'	-8.42	109.60	119.70
25	1	2531	C	P-O3'-C3'	-8.41	109.61	119.70
66	w2	69	C	P-O3'-C3'	-8.32	109.71	119.70
73	2	110	G	P-O3'-C3'	-8.32	109.71	119.70
73	2	521	C	N1-C2-O2	8.30	123.88	118.90
73	2	1134	U	P-O3'-C3'	-8.29	109.75	119.70
25	1	2296	G	P-O3'-C3'	-8.29	109.76	119.70
73	2	1169	C	P-O3'-C3'	-8.29	109.76	119.70
73	2	944	A	P-O3'-C3'	-8.28	109.76	119.70
73	2	1166	G	P-O3'-C3'	-8.27	109.77	119.70
73	2	604	C	P-O3'-C3'	-8.27	109.78	119.70
73	2	1130	C	P-O3'-C3'	-8.26	109.79	119.70
73	2	1386	C	P-O3'-C3'	-8.24	109.81	119.70
25	1	1814	A	P-O3'-C3'	-8.24	109.81	119.70
26	3	51	A	P-O3'-C3'	-8.19	109.87	119.70
73	2	1005	G	P-O3'-C3'	-8.17	109.90	119.70
25	1	2298	C	P-O3'-C3'	-8.16	109.90	119.70
73	2	1196	C	P-O3'-C3'	-8.16	109.91	119.70
73	2	900	C	N1-C2-O2	8.14	123.79	118.90
73	2	1167	C	P-O3'-C3'	-8.14	109.93	119.70
73	2	104	OMC	P-O3'-C3'	-8.11	109.97	119.70
25	1	2152	U	P-O3'-C3'	-8.10	109.98	119.70
25	1	1501	C	P-O3'-C3'	-8.06	110.02	119.70
66	w2	70	G	P-O3'-C3'	-8.06	110.03	119.70
73	2	106	C	P-O3'-C3'	-8.05	110.04	119.70
73	2	1388	C	P-O3'-C3'	-8.01	110.09	119.70
25	1	32	G	P-O3'-C3'	-7.99	110.12	119.70
25	1	552	A	P-O3'-C3'	-7.97	110.13	119.70
73	2	900	C	N3-C2-O2	-7.97	116.32	121.90
25	1	2211	C	P-O3'-C3'	-7.97	110.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	2	602	C	P-O3'-C3'	-7.97	110.14	119.70
66	w2	68	C	P-O3'-C3'	-7.93	110.18	119.70
73	2	900	C	C2-N1-C1'	7.93	127.52	118.80
73	2	10	G	P-O3'-C3'	-7.92	110.20	119.70
73	2	942	G	P-O3'-C3'	-7.88	110.24	119.70
73	2	7	G	P-O3'-C3'	-7.88	110.25	119.70
25	1	1866	G	P-O3'-C3'	-7.87	110.25	119.70
25	1	2232	C	P-O3'-C3'	-7.86	110.27	119.70
73	2	1006	C	P-O3'-C3'	-7.85	110.28	119.70
73	2	107	C	P-O3'-C3'	-7.85	110.28	119.70
25	1	2527	G	P-O3'-C3'	-7.83	110.30	119.70
73	2	854	G	P-O3'-C3'	-7.83	110.30	119.70
73	2	158	G	P-O3'-C3'	-7.82	110.32	119.70
25	1	1520	OMG	P-O3'-C3'	-7.80	110.34	119.70
25	1	2213	G	P-O3'-C3'	-7.79	110.35	119.70
25	1	1383	C	P-O3'-C3'	-7.79	110.36	119.70
25	1	568	U	P-O3'-C3'	-7.79	110.36	119.70
73	2	1197	C	P-O3'-C3'	-7.78	110.36	119.70
73	2	1170	G	P-O3'-C3'	-7.78	110.37	119.70
73	2	1136	U	P-O3'-C3'	-7.77	110.38	119.70
73	2	362	G	P-O3'-C3'	-7.74	110.41	119.70
25	1	569	G	P-O3'-C3'	-7.74	110.42	119.70
73	2	1164	A	P-O3'-C3'	-7.71	110.44	119.70
25	1	1832	G	P-O3'-C3'	-7.70	110.46	119.70
73	2	1387	C	P-O3'-C3'	-7.69	110.47	119.70
25	1	1813	G	P-O3'-C3'	-7.68	110.48	119.70
73	2	108	G	P-O3'-C3'	-7.68	110.48	119.70
73	2	150	C	P-O3'-C3'	-7.68	110.48	119.70
66	w2	72	C	P-O3'-C3'	-7.67	110.50	119.70
25	1	1858	G	P-O3'-C3'	-7.65	110.52	119.70
73	2	3	U	P-O3'-C3'	-7.64	110.53	119.70
66	w2	71	C	P-O3'-C3'	-7.63	110.54	119.70
25	1	1490	G	P-O3'-C3'	-7.62	110.56	119.70
25	1	1161	C	P-O3'-C3'	-7.61	110.56	119.70
73	2	1385	G	P-O3'-C3'	-7.59	110.59	119.70
73	2	151	A	P-O3'-C3'	-7.55	110.64	119.70
25	1	889	C	C6-N1-C1'	7.55	129.86	120.80
25	1	656	G	P-O3'-C3'	-7.52	110.68	119.70
73	2	948	C	P-O3'-C3'	-7.51	110.69	119.70
73	2	157	U	P-O3'-C3'	-7.51	110.69	119.70
73	2	900	C	C6-N1-C2	-7.48	117.31	120.30
25	1	2040	U	N3-C2-O2	-7.47	116.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	2	1391	G	P-O3'-C3'	-7.44	110.78	119.70
25	1	1483	G	P-O3'-C3'	-7.43	110.78	119.70
73	2	152	A	P-O3'-C3'	-7.42	110.79	119.70
25	1	2529	C	P-O3'-C3'	-7.42	110.80	119.70
73	2	1165	C	P-O3'-C3'	-7.41	110.81	119.70
25	1	2265	C	C6-N1-C2	-7.41	117.34	120.30
73	2	126	C	P-O3'-C3'	-7.34	110.89	119.70
25	1	2059	C	C2-N1-C1'	7.34	126.88	118.80
73	2	371	OMG	P-O3'-C3'	-7.34	110.89	119.70
25	1	2526	U	P-O3'-C3'	-7.32	110.92	119.70
25	1	1384	C	P-O3'-C3'	-7.30	110.94	119.70
73	2	591	G	P-O3'-C3'	-7.29	110.95	119.70
73	2	853	G	P-O3'-C3'	-7.29	110.95	119.70
73	2	588	C	P-O3'-C3'	-7.24	111.01	119.70
73	2	1013	G	P-O3'-C3'	-7.19	111.07	119.70
73	2	938	G	P-O3'-C3'	-7.17	111.09	119.70
25	1	1491	G	P-O3'-C3'	-7.16	111.11	119.70
25	1	2157	G	P-O3'-C3'	-7.15	111.12	119.70
25	1	2214	A	P-O3'-C3'	-7.15	111.12	119.70
25	1	2151	G	P-O3'-C3'	-7.12	111.15	119.70
73	2	852	G	P-O3'-C3'	-7.12	111.16	119.70
25	1	2235	A	P-O3'-C3'	-7.11	111.17	119.70
25	1	1484	A	P-O3'-C3'	-7.08	111.20	119.70
25	1	405	G	P-O3'-C3'	-7.07	111.22	119.70
73	2	929	U	P-O3'-C3'	-7.07	111.22	119.70
25	1	2386	U	P-O3'-C3'	-7.07	111.22	119.70
25	1	1824	OMC	P-O3'-C3'	-6.99	111.31	119.70
73	2	521	C	C6-N1-C1'	-6.99	112.41	120.80
25	1	2406	C	P-O3'-C3'	-6.98	111.32	119.70
73	2	1087	C	C2-N1-C1'	6.98	126.47	118.80
73	2	105	C	P-O3'-C3'	-6.97	111.33	119.70
73	2	462	U	C2-N1-C1'	6.95	126.04	117.70
25	1	1849	C	N3-C2-O2	-6.94	117.04	121.90
73	2	1163	C	P-O3'-C3'	-6.92	111.39	119.70
25	1	2212	G	P-O3'-C3'	-6.91	111.41	119.70
25	1	1812	G	P-O3'-C3'	-6.91	111.41	119.70
25	1	2059	C	N1-C2-O2	6.90	123.04	118.90
26	3	50	A	P-O3'-C3'	-6.89	111.43	119.70
73	2	1394	C	P-O3'-C3'	-6.89	111.43	119.70
73	2	596	G	P-O3'-C3'	-6.87	111.45	119.70
66	w2	73	A	P-O3'-C3'	-6.87	111.46	119.70
73	2	153	G	P-O3'-C3'	-6.86	111.46	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	1486	U	P-O3'-C3'	-6.85	111.47	119.70
25	1	300	C	N3-C2-O2	-6.84	117.11	121.90
25	1	1815	U	P-O3'-C3'	-6.84	111.49	119.70
25	1	2524	G	P-O3'-C3'	-6.83	111.50	119.70
73	2	849	G	P-O3'-C3'	-6.83	111.51	119.70
73	2	401	C	P-O3'-C3'	-6.83	111.51	119.70
73	2	1012	U	P-O3'-C3'	-6.81	111.53	119.70
73	2	1393	G	P-O3'-C3'	-6.81	111.53	119.70
25	1	1382	G	P-O3'-C3'	-6.80	111.54	119.70
25	1	2230	A	P-O3'-C3'	-6.80	111.54	119.70
25	1	2575	C	C2-N1-C1'	6.79	126.27	118.80
25	1	2155	C	P-O3'-C3'	-6.79	111.56	119.70
73	2	355	C	P-O3'-C3'	-6.79	111.56	119.70
25	1	2265	C	N1-C2-O2	6.79	122.97	118.90
25	1	2228	U	P-O3'-C3'	-6.76	111.59	119.70
73	2	356	C	P-O3'-C3'	-6.76	111.59	119.70
25	1	1904	U	P-O3'-C3'	-6.75	111.60	119.70
25	1	2265	C	N3-C2-O2	-6.74	117.18	121.90
73	2	358	A	P-O3'-C3'	-6.70	111.66	119.70
73	2	850	G	P-O3'-C3'	-6.70	111.66	119.70
25	1	300	C	N1-C2-O2	6.69	122.92	118.90
73	2	462	U	N1-C2-O2	6.69	127.48	122.80
25	1	2210	G	P-O3'-C3'	-6.67	111.70	119.70
73	2	858	A	P-O3'-C3'	-6.67	111.70	119.70
25	1	300	C	C6-N1-C2	-6.65	117.64	120.30
73	2	857	U	P-O3'-C3'	-6.65	111.72	119.70
25	1	2301	C	P-O3'-C3'	-6.64	111.73	119.70
73	2	1139	G	P-O3'-C3'	-6.64	111.73	119.70
25	1	1485	C	P-O3'-C3'	-6.63	111.74	119.70
25	1	2153	G	P-O3'-C3'	-6.62	111.75	119.70
25	1	1546	C	P-O3'-C3'	-6.61	111.77	119.70
25	1	300	C	C2-N1-C1'	6.61	126.07	118.80
25	1	1529	G	P-O3'-C3'	-6.61	111.77	119.70
25	1	1849	C	N3-C4-C5	-6.57	119.27	121.90
73	2	1258	C	C2-N1-C1'	6.57	126.03	118.80
25	1	2234	C	P-O3'-C3'	-6.55	111.84	119.70
25	1	2522	G	P-O3'-C3'	-6.52	111.87	119.70
25	1	2018	C	N3-C2-O2	-6.50	117.35	121.90
25	1	2299	G	P-O3'-C3'	-6.46	111.95	119.70
25	1	2149	C	P-O3'-C3'	-6.45	111.96	119.70
25	1	2300	G	P-O3'-C3'	-6.44	111.98	119.70
25	1	2304	U	P-O3'-C3'	-6.40	112.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	2	1171	C	P-O3'-C3'	-6.39	112.04	119.70
25	1	2209	C	P-O3'-C3'	-6.38	112.05	119.70
25	1	2233	A	P-O3'-C3'	-6.37	112.05	119.70
25	1	1808	A	P-O3'-C3'	-6.37	112.05	119.70
25	1	37	U	P-O3'-C3'	-6.37	112.06	119.70
25	1	2268	C	N3-C2-O2	-6.37	117.44	121.90
25	1	2040	U	N1-C2-N3	6.34	118.70	114.90
25	1	1620	C	C6-N1-C2	-6.33	117.77	120.30
25	1	2295	U	N3-C2-O2	-6.33	117.77	122.20
27	42	104	A	O5'-P-OP1	-6.33	100.00	105.70
25	1	567	C	P-O3'-C3'	-6.32	112.11	119.70
73	2	928	C	P-O3'-C3'	-6.32	112.12	119.70
25	1	1544	G	P-O3'-C3'	-6.32	112.12	119.70
25	1	1162	U	P-O3'-C3'	-6.31	112.13	119.70
25	1	112	C	C2-N1-C1'	6.30	125.73	118.80
25	1	178	G	N3-C4-N9	6.30	129.78	126.00
25	1	1482	G	P-O3'-C3'	-6.30	112.14	119.70
73	2	851	G	P-O3'-C3'	-6.29	112.15	119.70
25	1	1809	C	P-O3'-C3'	-6.29	112.15	119.70
73	2	624	G	N3-C4-N9	6.26	129.75	126.00
73	2	1095	C	P-O3'-C3'	-6.26	112.19	119.70
27	42	98	C	C2-N1-C1'	6.25	125.68	118.80
25	1	1816	C	P-O3'-C3'	-6.24	112.21	119.70
73	2	589	G	P-O3'-C3'	-6.24	112.21	119.70
25	1	2158	C	P-O3'-C3'	-6.24	112.22	119.70
73	2	1258	C	N1-C2-O2	6.24	122.64	118.90
25	1	1849	C	C4-C5-C6	6.23	120.51	117.40
26	3	28	C	P-O3'-C3'	-6.22	112.23	119.70
25	1	1489	G	P-O3'-C3'	-6.22	112.23	119.70
25	1	1539	A	P-O3'-C3'	-6.22	112.24	119.70
73	2	947	U	P-O3'-C3'	-6.21	112.25	119.70
2	N1	135	LEU	CA-CB-CG	6.20	129.56	115.30
73	2	462	U	N3-C2-O2	-6.20	117.86	122.20
73	2	610	C	N3-C4-C5	6.19	124.38	121.90
25	1	2150	C	P-O3'-C3'	-6.18	112.28	119.70
25	1	1861	C	P-O3'-C3'	-6.16	112.31	119.70
25	1	2546	C	C2-N1-C1'	6.14	125.56	118.80
25	1	1252	C	O4'-C1'-N1	6.14	113.11	108.20
25	1	570	G	P-O3'-C3'	-6.13	112.35	119.70
25	1	1163	G	P-O3'-C3'	-6.12	112.36	119.70
25	1	2354	U	P-O3'-C3'	6.11	127.03	119.70
73	2	1201	A	P-O3'-C3'	-6.11	112.37	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	2	491	G	C4-N9-C1'	6.10	134.43	126.50
25	1	1871	C	C6-N1-C2	-6.09	117.86	120.30
73	2	1202	G	P-O3'-C3'	-6.08	112.40	119.70
25	1	388	C	P-O3'-C3'	-6.05	112.44	119.70
25	1	1903	U	P-O3'-C3'	-6.01	112.48	119.70
25	1	1179	C	C2-N1-C1'	6.01	125.41	118.80
25	1	429	G	N7-C8-N9	6.01	116.10	113.10
25	1	1905	G	P-O3'-C3'	-6.00	112.50	119.70
73	2	407	C	C2-N1-C1'	6.00	125.40	118.80
25	1	2265	C	C2-N1-C1'	5.98	125.38	118.80
25	1	1602	C	C6-N1-C2	-5.96	117.92	120.30
25	1	2231	C	P-O3'-C3'	-5.94	112.57	119.70
66	w2	75	C	N3-C2-O2	-5.94	117.74	121.90
73	2	624	G	N3-C4-C5	-5.94	125.63	128.60
25	1	2533	U	P-O3'-C3'	-5.94	112.57	119.70
73	2	686	C	C2-N1-C1'	5.94	125.33	118.80
25	1	1871	C	C2-N1-C1'	5.93	125.33	118.80
73	2	1089	G	O4'-C1'-N9	5.93	112.94	108.20
25	1	399	G	N3-C4-C5	-5.93	125.64	128.60
73	2	601	C	P-O3'-C3'	-5.92	112.60	119.70
73	2	354	C	P-O3'-C3'	-5.91	112.60	119.70
73	2	357	A	P-O3'-C3'	-5.91	112.61	119.70
25	1	2018	C	N1-C2-O2	5.91	122.44	118.90
25	1	551	G	P-O3'-C3'	-5.90	112.62	119.70
25	1	2422	C	O4'-C1'-N1	5.90	112.92	108.20
25	1	1541	G	P-O3'-C3'	-5.90	112.62	119.70
25	1	35	C	P-O3'-C3'	-5.89	112.63	119.70
25	1	41	C	P-O3'-C3'	-5.88	112.64	119.70
73	2	368	C	P-O3'-C3'	-5.88	112.65	119.70
25	1	34	A	P-O3'-C3'	-5.87	112.66	119.70
73	2	592	C	P-O3'-C3'	-5.85	112.68	119.70
25	1	2018	C	C6-N1-C2	-5.84	117.96	120.30
25	1	36	U	P-O3'-C3'	-5.84	112.69	119.70
73	2	1199	C	C6-N1-C2	-5.84	117.96	120.30
25	1	1277	A	O4'-C1'-N9	5.82	112.86	108.20
73	2	607	C	P-O3'-C3'	-5.82	112.72	119.70
25	1	638	U	C2-N1-C1'	5.81	124.67	117.70
25	1	2217	U	P-O3'-C3'	-5.80	112.73	119.70
73	2	587	G	P-O3'-C3'	-5.80	112.74	119.70
25	1	589	C	P-O3'-C3'	5.80	126.66	119.70
25	1	2546	C	N1-C2-O2	5.79	122.37	118.90
73	2	1087	C	C6-N1-C1'	-5.79	113.86	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	2543	C	C5-C6-N1	5.78	123.89	121.00
26	3	94	U	N3-C2-O2	-5.78	118.16	122.20
73	2	610	C	N1-C2-O2	5.78	122.37	118.90
73	2	621	G	N3-C4-C5	-5.78	125.71	128.60
73	2	235	U	C2-N1-C1'	5.76	124.62	117.70
25	1	156	G	O4'-C1'-N9	5.75	112.80	108.20
73	2	491	G	C8-N9-C1'	-5.73	119.55	127.00
73	2	935	A	P-O3'-C3'	-5.73	112.83	119.70
25	1	2499	G	N3-C4-N9	5.71	129.43	126.00
25	1	2499	G	N3-C4-C5	-5.69	125.75	128.60
73	2	535	A	O4'-C1'-N9	5.69	112.75	108.20
25	1	2268	C	C6-N1-C2	-5.68	118.03	120.30
25	1	2215	G	P-O3'-C3'	-5.67	112.90	119.70
73	2	1282	C	N1-C2-O2	5.67	122.30	118.90
25	1	575	G	P-O3'-C3'	-5.66	112.90	119.70
65	p2	60	CYS	CA-CB-SG	5.66	124.19	114.00
73	2	1195	C	P-O3'-C3'	-5.66	112.91	119.70
25	1	1261	C	N1-C2-O2	5.64	122.28	118.90
25	1	611	G	N3-C4-N9	5.63	129.38	126.00
27	42	99	C	C2-N1-C1'	5.63	124.99	118.80
25	1	1542	C	P-O3'-C3'	-5.63	112.94	119.70
73	2	593	C	P-O3'-C3'	-5.62	112.95	119.70
73	2	804	C	C6-N1-C2	-5.62	118.05	120.30
23	L1	34	LEU	CA-CB-CG	5.62	128.22	115.30
25	1	1850	A	P-O3'-C3'	-5.62	112.96	119.70
25	1	1863	G	P-O3'-C3'	-5.60	112.98	119.70
73	2	855	A	P-O3'-C3'	-5.58	113.00	119.70
25	1	1760	G	O4'-C1'-N9	5.57	112.66	108.20
73	2	755	A	O4'-C1'-N9	5.57	112.65	108.20
25	1	1865	C	P-O3'-C3'	-5.57	113.02	119.70
25	1	802	C	N1-C2-O2	5.55	122.23	118.90
25	1	2258	C	N1-C2-O2	5.55	122.23	118.90
73	2	280	U	N3-C2-O2	-5.54	118.32	122.20
25	1	1208	C	C6-N1-C2	-5.53	118.09	120.30
73	2	1282	C	C2-N1-C1'	5.52	124.87	118.80
25	1	112	C	C6-N1-C2	-5.52	118.09	120.30
25	1	545	G	O4'-C1'-N9	5.51	112.61	108.20
73	2	112	C	P-O3'-C3'	-5.50	113.09	119.70
73	2	856	G	P-O3'-C3'	-5.50	113.10	119.70
73	2	1356	G	N3-C4-N9	5.49	129.29	126.00
73	2	791	C	C6-N1-C2	-5.49	118.10	120.30
25	1	1864	G	P-O3'-C3'	-5.48	113.12	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	2	149	C	P-O3'-C3'	-5.48	113.12	119.70
25	1	2305	U	P-O3'-C3'	-5.48	113.13	119.70
25	1	2258	C	N3-C2-O2	-5.47	118.07	121.90
25	1	396	A2M	P-O3'-C3'	-5.47	113.14	119.70
25	1	178	G	N3-C4-C5	-5.46	125.87	128.60
25	1	33	A	P-O3'-C3'	-5.46	113.15	119.70
25	1	611	G	N3-C4-C5	-5.45	125.88	128.60
73	2	113	G	P-O3'-C3'	-5.45	113.16	119.70
25	1	658	U	P-O3'-C3'	-5.45	113.16	119.70
25	1	1160	A	P-O3'-C3'	-5.45	113.16	119.70
25	1	886	C	C6-N1-C2	-5.42	118.13	120.30
25	1	2208	G	P-O3'-C3'	-5.42	113.19	119.70
73	2	1258	C	N3-C2-O2	-5.42	118.11	121.90
73	2	1421	G	N3-C4-C5	5.42	131.31	128.60
22	E1	139	LEU	CA-CB-CG	5.42	127.76	115.30
25	1	1792	G	O4'-C1'-N9	5.42	112.53	108.20
73	2	1097	G	P-O3'-C3'	-5.41	113.20	119.70
25	1	2040	U	C4-C5-C6	5.40	122.94	119.70
25	1	2545	C	C6-N1-C2	-5.40	118.14	120.30
73	2	717	C	C2-N1-C1'	5.39	124.73	118.80
25	1	2528	C	P-O3'-C3'	-5.39	113.23	119.70
25	1	889	C	N1-C2-O2	-5.39	115.67	118.90
25	1	2059	C	C6-N1-C1'	-5.38	114.34	120.80
25	1	429	G	C5-N7-C8	-5.38	101.61	104.30
25	1	2129	G	C4-N9-C1'	5.38	133.50	126.50
25	1	2538	A	P-O3'-C3'	-5.38	113.24	119.70
25	1	2268	C	C2-N1-C1'	5.38	124.72	118.80
73	2	1154	C	C6-N1-C2	-5.37	118.15	120.30
25	1	1856	G	N3-C4-N9	5.37	129.22	126.00
25	1	2596	C	N1-C2-O2	5.37	122.12	118.90
25	1	1502	U	P-O3'-C3'	-5.36	113.27	119.70
25	1	989	G	N3-C4-N9	5.36	129.22	126.00
73	2	521	C	N3-C2-O2	-5.35	118.15	121.90
25	1	1894	C	C6-N1-C2	-5.35	118.16	120.30
25	1	2297	U	P-O3'-C3'	-5.34	113.29	119.70
25	1	2513	G	N3-C4-C5	-5.33	125.94	128.60
25	1	2268	C	N1-C2-O2	5.32	122.09	118.90
68	E	74	C	C6-N1-C2	-5.31	118.17	120.30
25	1	490	G	C6-C5-N7	-5.30	127.22	130.40
56	f2	9	PHE	C-N-CA	5.30	134.94	121.70
25	1	518	C	C6-N1-C2	-5.29	118.18	120.30
73	2	936	A	P-O3'-C3'	-5.29	113.35	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	1882	OMG	P-O3'-C3'	-5.29	113.35	119.70
27	42	98	C	N3-C2-O2	-5.29	118.20	121.90
25	1	1538	C	P-O3'-C3'	-5.28	113.37	119.70
25	1	2258	C	C2-N1-C1'	5.27	124.60	118.80
73	2	381	C	N3-C2-O2	-5.27	118.21	121.90
25	1	2289	C	C6-N1-C2	-5.27	118.19	120.30
25	1	376	C	C6-N1-C2	-5.27	118.19	120.30
26	3	77	U	N3-C2-O2	-5.26	118.52	122.20
25	1	1381	C	P-O3'-C3'	-5.25	113.40	119.70
25	1	576	G	P-O3'-C3'	-5.25	113.41	119.70
25	1	165	G	N3-C4-C5	5.24	131.22	128.60
73	2	83	G	P-O3'-C3'	-5.23	113.42	119.70
25	1	545	G	C4-N9-C1'	5.23	133.30	126.50
25	1	632	G	P-O3'-C3'	5.23	125.97	119.70
25	1	1849	C	N1-C2-N3	5.23	122.86	119.20
25	1	1261	C	N3-C2-O2	-5.22	118.24	121.90
25	1	186	A	O4'-C1'-N9	5.22	112.38	108.20
73	2	605	G	P-O3'-C3'	-5.22	113.43	119.70
25	1	2575	C	C6-N1-C2	-5.22	118.21	120.30
25	1	387	U	P-O3'-C3'	-5.21	113.44	119.70
25	1	2543	C	C6-N1-C2	-5.21	118.21	120.30
73	2	1199	C	N3-C2-O2	-5.21	118.25	121.90
25	1	2523	C	P-O3'-C3'	-5.21	113.44	119.70
25	1	1006	G	O4'-C1'-N9	5.21	112.37	108.20
25	1	2575	C	O4'-C1'-N1	5.20	112.36	108.20
25	1	1871	C	N3-C2-O2	-5.20	118.26	121.90
26	3	94	U	C2-N1-C1'	5.20	123.94	117.70
25	1	1178	U	N3-C2-O2	-5.19	118.57	122.20
25	1	724	C	C6-N1-C2	-5.19	118.22	120.30
25	1	2019	C	C6-N1-C2	-5.18	118.23	120.30
25	1	1924	G	N3-C4-N9	5.18	129.11	126.00
73	2	984	C	C6-N1-C2	-5.17	118.23	120.30
25	1	1330	G	N3-C4-N9	5.17	129.10	126.00
25	1	1545	G	P-O3'-C3'	-5.17	113.50	119.70
25	1	989	G	C6-C5-N7	-5.17	127.30	130.40
73	2	364	G	P-O3'-C3'	-5.16	113.51	119.70
73	2	1305	C	C6-N1-C2	-5.16	118.24	120.30
25	1	2581	C	C2-N1-C1'	5.16	124.47	118.80
25	1	126	U	N3-C2-O2	-5.15	118.59	122.20
45	T2	81	ARG	CA-CB-CG	5.15	124.73	113.40
25	1	2596	C	C2-N1-C1'	5.14	124.46	118.80
25	1	185	C	C6-N1-C2	-5.14	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	376	C	C2-N1-C1’	5.13	124.44	118.80
25	1	802	C	N3-C2-O2	-5.13	118.31	121.90
25	1	1831	C	P-O3’-C3’	-5.13	113.55	119.70
25	1	2550	C	N3-C2-O2	-5.13	118.31	121.90
25	1	2418	G	N3-C4-C5	-5.12	126.04	128.60
25	1	1488	C	P-O3’-C3’	-5.12	113.56	119.70
25	1	2628	C	N1-C2-O2	5.11	121.97	118.90
4	D1	148	LEU	CA-CB-CG	-5.10	103.58	115.30
25	1	1280	C	C2-N1-C1’	5.10	124.41	118.80
25	1	2367	A	P-O3’-C3’	-5.09	113.59	119.70
73	2	280	U	C2-N1-C1’	5.08	123.79	117.70
25	1	2596	C	C6-N1-C2	-5.06	118.28	120.30
25	1	763	C	C5-C6-N1	5.05	123.53	121.00
73	2	1129	G	N3-C4-C5	-5.05	126.07	128.60
9	B1	31	ILE	C-N-CA	5.05	134.33	121.70
25	1	1532	A	P-O3’-C3’	-5.05	113.64	119.70
25	1	438	C	C6-N1-C2	-5.03	118.29	120.30
25	1	178	G	C4-N9-C1’	5.02	133.03	126.50
25	1	574	A	P-O3’-C3’	-5.01	113.69	119.70
25	1	638	U	N1-C2-O2	5.01	126.31	122.80
25	1	2415	C	C2-N1-C1’	5.01	124.31	118.80
34	H2	159	GLU	CA-CB-CG	5.01	124.42	113.40
73	2	1199	C	N1-C2-O2	5.01	121.91	118.90
25	1	2628	C	C2-N1-C1’	5.01	124.31	118.80
25	1	1537	G	C8-N9-C4	-5.00	104.40	106.40

There are no chirality outliers.

There are no planarity outliers.

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	
1	T1	102/139 (73%)	97 (95%)	5 (5%)	0	100	100
2	N1	150/154 (97%)	142 (95%)	8 (5%)	0	100	100
3	J1	164/189 (87%)	153 (93%)	11 (7%)	0	100	100
4	D1	174/217 (80%)	163 (94%)	11 (6%)	0	100	100
5	X1	140/143 (98%)	130 (93%)	10 (7%)	0	100	100
6	S1	131/154 (85%)	113 (86%)	18 (14%)	0	100	100
7	Q1	119/158 (75%)	108 (91%)	11 (9%)	0	100	100
8	C1	210/242 (87%)	195 (93%)	15 (7%)	0	100	100
9	B1	216/248 (87%)	207 (96%)	9 (4%)	0	100	100
10	b1	77/124 (62%)	71 (92%)	6 (8%)	0	100	100
11	a1	95/109 (87%)	90 (95%)	5 (5%)	0	100	100
12	V1	80/89 (90%)	72 (90%)	8 (10%)	0	100	100
13	R1	93/137 (68%)	87 (94%)	6 (6%)	0	100	100
14	K1	79/134 (59%)	70 (89%)	9 (11%)	0	100	100
15	I1	159/174 (91%)	147 (92%)	12 (8%)	0	100	100
16	e1	31/69 (45%)	29 (94%)	2 (6%)	0	100	100
17	H1	148/190 (78%)	133 (90%)	15 (10%)	0	100	100
18	n1	22/41 (54%)	22 (100%)	0	0	100	100
19	c1	51/64 (80%)	47 (92%)	4 (8%)	0	100	100
20	O1	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
21	W1	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
22	E1	256/268 (96%)	234 (91%)	22 (9%)	0	100	100
23	L1	179/199 (90%)	169 (94%)	10 (6%)	0	100	100
24	U1	68/126 (54%)	63 (93%)	5 (7%)	0	100	100
28	A2	248/251 (99%)	237 (96%)	11 (4%)	0	100	100
29	B2	376/379 (99%)	357 (95%)	19 (5%)	0	100	100
30	C2	312/316 (99%)	295 (95%)	17 (5%)	0	100	100
31	D2	264/297 (89%)	247 (94%)	17 (6%)	0	100	100
32	F2	212/235 (90%)	209 (99%)	3 (1%)	0	100	100
33	G2	178/225 (79%)	173 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	H2	182/185 (98%)	172 (94%)	10 (6%)	0	100	100
35	I2	196/210 (93%)	187 (95%)	9 (5%)	0	100	100
36	J2	158/173 (91%)	144 (91%)	14 (9%)	0	100	100
37	L2	185/234 (79%)	183 (99%)	2 (1%)	0	100	100
38	M2	126/131 (96%)	115 (91%)	11 (9%)	0	100	100
39	N2	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
40	O2	193/197 (98%)	186 (96%)	7 (4%)	0	100	100
41	P2	152/164 (93%)	143 (94%)	9 (6%)	0	100	100
42	Q2	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
43	R2	175/196 (89%)	166 (95%)	9 (5%)	0	100	100
44	S2	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
45	T2	149/159 (94%)	145 (97%)	4 (3%)	0	100	100
46	U2	98/171 (57%)	90 (92%)	8 (8%)	0	100	100
47	V2	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
48	X2	114/141 (81%)	109 (96%)	5 (4%)	0	100	100
49	Y2	131/135 (97%)	126 (96%)	5 (4%)	0	100	100
50	Z2	125/135 (93%)	115 (92%)	10 (8%)	0	100	100
51	a2	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
52	b2	54/62 (87%)	54 (100%)	0	0	100	100
53	c2	98/109 (90%)	97 (99%)	1 (1%)	0	100	100
54	d2	90/106 (85%)	81 (90%)	9 (10%)	0	100	100
55	e2	124/136 (91%)	119 (96%)	5 (4%)	0	100	100
56	f2	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
57	g2	97/120 (81%)	94 (97%)	3 (3%)	0	100	100
58	h2	116/124 (94%)	114 (98%)	2 (2%)	0	100	100
59	i2	81/90 (90%)	76 (94%)	5 (6%)	0	100	100
60	j2	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
61	k2	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
62	l2	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
63	m2	49/127 (39%)	46 (94%)	3 (6%)	0	100	100
64	o2	92/106 (87%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	p2	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
67	W2	63/102 (62%)	59 (94%)	4 (6%)	0	100	100
69	d1	46/137 (34%)	40 (87%)	6 (13%)	0	100	100
70	F1	157/190 (83%)	127 (81%)	27 (17%)	3 (2%)	8	14
71	Y1	87/132 (66%)	76 (87%)	10 (12%)	1 (1%)	14	25
72	G1	177/248 (71%)	134 (76%)	37 (21%)	6 (3%)	3	5
74	A1	192/245 (78%)	185 (96%)	7 (4%)	0	100	100
All	All	9329/10892 (86%)	8754 (94%)	565 (6%)	10 (0%)	54	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
72	G1	103	ILE
72	G1	114	ALA
72	G1	106	CYS
70	F1	34	PHE
72	G1	65	GLN
72	G1	110	PRO
70	F1	71	LYS
70	F1	160	ALA
71	Y1	34	GLU
72	G1	77	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T1	78/115 (68%)	76 (97%)	2 (3%)	46	66
2	N1	123/130 (95%)	123 (100%)	0	100	100
3	J1	141/164 (86%)	140 (99%)	1 (1%)	84	89
4	D1	142/182 (78%)	142 (100%)	0	100	100
5	X1	113/114 (99%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S1	112/131 (86%)	109 (97%)	3 (3%)	44	65
7	Q1	101/130 (78%)	101 (100%)	0	100	100
8	C1	176/201 (88%)	176 (100%)	0	100	100
9	B1	196/220 (89%)	195 (100%)	1 (0%)	88	92
10	b1	70/112 (62%)	70 (100%)	0	100	100
11	a1	90/103 (87%)	90 (100%)	0	100	100
12	V1	62/72 (86%)	62 (100%)	0	100	100
13	R1	81/123 (66%)	80 (99%)	1 (1%)	71	82
14	K1	73/119 (61%)	73 (100%)	0	100	100
15	I1	138/148 (93%)	138 (100%)	0	100	100
16	e1	30/58 (52%)	30 (100%)	0	100	100
17	H1	116/170 (68%)	115 (99%)	1 (1%)	78	87
18	n1	21/38 (55%)	21 (100%)	0	100	100
19	c1	49/57 (86%)	48 (98%)	1 (2%)	55	72
20	O1	91/113 (80%)	91 (100%)	0	100	100
21	W1	114/115 (99%)	114 (100%)	0	100	100
22	E1	225/232 (97%)	225 (100%)	0	100	100
23	L1	155/173 (90%)	153 (99%)	2 (1%)	69	81
24	U1	68/110 (62%)	68 (100%)	0	100	100
28	A2	189/192 (98%)	189 (100%)	0	100	100
29	B2	312/313 (100%)	312 (100%)	0	100	100
30	C2	261/263 (99%)	260 (100%)	1 (0%)	91	93
31	D2	210/242 (87%)	209 (100%)	1 (0%)	88	92
32	F2	184/204 (90%)	183 (100%)	1 (0%)	88	92
33	G2	159/198 (80%)	158 (99%)	1 (1%)	86	90
34	H2	160/164 (98%)	160 (100%)	0	100	100
35	I2	166/177 (94%)	166 (100%)	0	100	100
36	J2	137/149 (92%)	136 (99%)	1 (1%)	84	89
37	L2	159/197 (81%)	159 (100%)	0	100	100
38	M2	103/111 (93%)	102 (99%)	1 (1%)	76	85
39	N2	174/175 (99%)	173 (99%)	1 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	O2	164/165 (99%)	164 (100%)	0	100	100
41	P2	130/139 (94%)	130 (100%)	0	100	100
42	Q2	154/155 (99%)	154 (100%)	0	100	100
43	R2	149/167 (89%)	144 (97%)	5 (3%)	37	58
44	S2	147/154 (96%)	146 (99%)	1 (1%)	84	89
45	T2	126/133 (95%)	126 (100%)	0	100	100
46	U2	87/153 (57%)	87 (100%)	0	100	100
47	V2	112/114 (98%)	111 (99%)	1 (1%)	78	87
48	X2	104/123 (85%)	104 (100%)	0	100	100
49	Y2	114/115 (99%)	114 (100%)	0	100	100
50	Z2	101/119 (85%)	101 (100%)	0	100	100
51	a2	126/127 (99%)	126 (100%)	0	100	100
52	b2	51/57 (90%)	51 (100%)	0	100	100
53	c2	84/92 (91%)	84 (100%)	0	100	100
54	d2	78/92 (85%)	78 (100%)	0	100	100
55	e2	112/120 (93%)	112 (100%)	0	100	100
56	f2	102/103 (99%)	102 (100%)	0	100	100
57	g2	87/100 (87%)	87 (100%)	0	100	100
58	h2	102/107 (95%)	102 (100%)	0	100	100
59	i2	72/78 (92%)	72 (100%)	0	100	100
60	j2	70/74 (95%)	70 (100%)	0	100	100
61	k2	56/68 (82%)	56 (100%)	0	100	100
62	l2	46/48 (96%)	45 (98%)	1 (2%)	52	70
63	m2	46/110 (42%)	45 (98%)	1 (2%)	52	70
64	o2	81/93 (87%)	81 (100%)	0	100	100
65	p2	71/73 (97%)	69 (97%)	2 (3%)	43	63
67	W2	58/92 (63%)	58 (100%)	0	100	100
69	d1	41/116 (35%)	40 (98%)	1 (2%)	49	68
70	F1	132/157 (84%)	123 (93%)	9 (7%)	16	28
71	Y1	77/113 (68%)	75 (97%)	2 (3%)	46	66
72	G1	153/213 (72%)	152 (99%)	1 (1%)	84	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	A1	168/217 (77%)	167 (99%)	1 (1%)	86	90
All	All	7980/9302 (86%)	7936 (99%)	44 (1%)	86	90

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T1	91	HIS
1	T1	101	ARG
3	J1	126	HIS
6	S1	12	ARG
6	S1	16	ARG
6	S1	48	LYS
9	B1	99	ASN
13	R1	28	ASP
17	H1	113	SER
19	c1	6	ASN
23	L1	32	ARG
23	L1	111	ARG
30	C2	144	VAL
31	D2	70	LYS
32	F2	66	LYS
33	G2	90	ARG
36	J2	7	ASN
38	M2	60	GLN
39	N2	96	ARG
43	R2	8	LYS
43	R2	119	LEU
43	R2	151	LEU
43	R2	154	LYS
43	R2	165	LYS
44	S2	167	ARG
47	V2	14	LYS
62	l2	46	ARG
63	m2	91	GLN
65	p2	3	LYS
65	p2	80	ARG
69	d1	123	CYS
70	F1	23	LEU
70	F1	57	ARG
70	F1	58	LEU
70	F1	63	MET
70	F1	67	ARG

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Mol	Chain	Res	Type
70	F1	79	VAL
70	F1	125	VAL
70	F1	142	THR
70	F1	174	TYR
71	Y1	37	GLU
71	Y1	69	THR
72	G1	7	CYS
74	A1	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
3	J1	112	GLN
4	D1	168	HIS
7	Q1	101	GLN
8	C1	194	GLN
9	B1	81	ASN
9	B1	108	HIS
9	B1	232	HIS
13	R1	77	GLN
21	W1	18	GLN
21	W1	59	ASN
22	E1	69	ASN
29	B2	71	GLN
29	B2	162	HIS
29	B2	354	GLN
30	C2	210	ASN
30	C2	274	GLN
33	G2	62	ASN
35	I2	51	HIS
42	Q2	87	ASN
45	T2	75	GLN
45	T2	105	HIS
51	a2	86	GLN
70	F1	37	HIS
70	F1	68	ASN
70	F1	189	ASN
71	Y1	14	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	1	2419/2707 (89%)	410 (16%)	24 (0%)
26	3	116/120 (96%)	16 (13%)	2 (1%)
27	42	136/139 (97%)	35 (25%)	2 (1%)
66	w2	12/14 (85%)	4 (33%)	0
68	E	2/3 (66%)	1 (50%)	0
73	2	1329/1452 (91%)	304 (22%)	17 (1%)
All	All	4014/4435 (90%)	770 (19%)	45 (1%)

All (770) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	1	5	G
25	1	21	G
25	1	39	A
25	1	42	A
25	1	48	G
25	1	56	C
25	1	58	G
25	1	59	A
25	1	64	A
25	1	65	A
25	1	71	C
25	1	73	G
25	1	84	U
25	1	89	G
25	1	90	C
25	1	106	A
25	1	107	G
25	1	108	C
25	1	110	C
25	1	117	A
25	1	120	G
25	1	122	G
25	1	127	G
25	1	128	U
25	1	156	G
25	1	157	G
25	1	165	G
25	1	166	G
25	1	171	C
25	1	176	G
25	1	180	G
25	1	184	G

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Mol	Chain	Res	Type
25	1	185	C
25	1	186	A
25	1	187	A
25	1	188	G
25	1	192	C
25	1	198	G
25	1	201	G
25	1	219	C
25	1	222	G
25	1	239	U
25	1	248	A
25	1	250	G
25	1	280	G
25	1	288	A
25	1	301	C
25	1	313	OMG
25	1	321	U
25	1	326	A
25	1	327	G
25	1	341	C
25	1	347	A
25	1	348	A
25	1	349	A
25	1	350	G
25	1	351	A
25	1	375	C
25	1	376	C
25	1	377	G
25	1	378	C
25	1	383	C
25	1	396	A2M
25	1	400	A
25	1	407	A
25	1	424	A
25	1	428	C
25	1	429	G
25	1	431	G
25	1	448	A
25	1	458	A
25	1	459	G
25	1	460	A
25	1	461	C

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Mol	Chain	Res	Type
25	1	462	G
25	1	463	C
25	1	476	G
25	1	482	C
25	1	485	C
25	1	490	G
25	1	493	C
25	1	501	G
25	1	516	G
25	1	522	A
25	1	533	U
25	1	565	G
25	1	573	G
25	1	574	A
25	1	577	C
25	1	585	G
25	1	590	U
25	1	595	C
25	1	611	G
25	1	612	A
25	1	623	G
25	1	630	A
25	1	632	G
25	1	633	A
25	1	637	A
25	1	639	C
25	1	640	G
25	1	641	A
25	1	653	G
25	1	660	G
25	1	675	C
25	1	676	C
25	1	690	G
25	1	705	C
25	1	722	G
25	1	759	A
25	1	761	C
25	1	776	C
25	1	790	G
25	1	791	C
25	1	793	U
25	1	798	G

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Mol	Chain	Res	Type
25	1	800	G
25	1	801	G
25	1	803	G
25	1	804	G
25	1	806	C
25	1	807	G
25	1	808	A
25	1	813	G
25	1	826	G
25	1	840	G
25	1	853	G
25	1	868	A
25	1	869	C
25	1	889	C
25	1	906	G
25	1	907	C
25	1	908	G
25	1	911	G
25	1	912	G
25	1	915	G
25	1	989	G
25	1	990	G
25	1	992	C
25	1	1004	U
25	1	1006	G
25	1	1008	G
25	1	1012	G
25	1	1014	C
25	1	1015	G
25	1	1016	G
25	1	1017	A
25	1	1018	G
25	1	1029	G
25	1	1030	C
25	1	1031	G
25	1	1042	G
25	1	1045	C
25	1	1046	G
25	1	1047	C
25	1	1050	C
25	1	1061	C
25	1	1066	G

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Mol	Chain	Res	Type
25	1	1072	C
25	1	1074	G
25	1	1080	G
25	1	1106	C
25	1	1108	G
25	1	1118	G
25	1	1121	OMG
25	1	1124	C
25	1	1137	G
25	1	1149	C
25	1	1158	G
25	1	1164	A
25	1	1166	G
25	1	1167	G
25	1	1186	G
25	1	1203	G
25	1	1205	U
25	1	1230	A
25	1	1232	A
25	1	1236	G
25	1	1238	A
25	1	1241	G
25	1	1244	C
25	1	1246	U
25	1	1247	G
25	1	1248	C
25	1	1252	C
25	1	1253	C
25	1	1254	C
25	1	1256	U
25	1	1259	A
25	1	1261	C
25	1	1265	G
25	1	1277	A
25	1	1291	G
25	1	1292	G
25	1	1314	C
25	1	1322	C
25	1	1331	G
25	1	1337	C
25	1	1349	C
25	1	1358	G

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Mol	Chain	Res	Type
25	1	1380	A
25	1	1381	C
25	1	1382	G
25	1	1388	C
25	1	1405	G
25	1	1411	G
25	1	1418	G
25	1	1439	A
25	1	1452	C
25	1	1472	G
25	1	1473	A
25	1	1481	A
25	1	1487	C
25	1	1488	C
25	1	1502	U
25	1	1508	G
25	1	1509	C
25	1	1510	G
25	1	1515	C
25	1	1516	G
25	1	1537	G
25	1	1538	C
25	1	1565	G
25	1	1566	G
25	1	1588	G
25	1	1589	G
25	1	1599	G
25	1	1600	A
25	1	1606	C
25	1	1609	G
25	1	1610	G
25	1	1619	A
25	1	1628	U
25	1	1646	A
25	1	1647	G
25	1	1663	U
25	1	1675	A
25	1	1694	A
25	1	1696	C
25	1	1712	U
25	1	1719	A
25	1	1731	A

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Mol	Chain	Res	Type
25	1	1733	G
25	1	1736	G
25	1	1737	G
25	1	1739	A
25	1	1740	G
25	1	1742	A
25	1	1759	G
25	1	1760	G
25	1	1766	A
25	1	1767	A
25	1	1768	A2M
25	1	1769	U
25	1	1775	OMG
25	1	1791	C
25	1	1797	U
25	1	1800	A
25	1	1801	U
25	1	1802	G
25	1	1812	G
25	1	1821	U
25	1	1823	U
25	1	1852	C
25	1	1860	A
25	1	1861	C
25	1	1862	G
25	1	1872	C
25	1	1880	G
25	1	1884	C
25	1	1888	A
25	1	1889	A
25	1	1890	G
25	1	1891	A
25	1	1898	U
25	1	1905	G
25	1	1906	A
25	1	1908	OMU
25	1	1922	G
25	1	1931	G
25	1	1992	C
25	1	1999	C
25	1	2004	G
25	1	2007	C

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Mol	Chain	Res	Type
25	1	2011	C
25	1	2012	G
25	1	2016	A
25	1	2019	C
25	1	2029	G
25	1	2030	G
25	1	2037	G
25	1	2049	G
25	1	2050	C
25	1	2060	A
25	1	2075	U
25	1	2078	C
25	1	2079	A
25	1	2088	U
25	1	2091	G
25	1	2092	C
25	1	2096	G
25	1	2097	A
25	1	2098	C
25	1	2112	G
25	1	2113	G
25	1	2114	A
25	1	2117	A
25	1	2127	A
25	1	2137	G
25	1	2139	C
25	1	2151	G
25	1	2163	G
25	1	2175	G
25	1	2176	G
25	1	2185	A
25	1	2196	C
25	1	2200	G
25	1	2202	C
25	1	2213	G
25	1	2218	G
25	1	2222	G
25	1	2223	A
25	1	2224	A
25	1	2233	A
25	1	2236	G
25	1	2239	A

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Mol	Chain	Res	Type
25	1	2241	A
25	1	2243	C
25	1	2251	U
25	1	2264	C
25	1	2267	G
25	1	2269	A
25	1	2275	G
25	1	2282	U
25	1	2293	G
25	1	2294	A
25	1	2297	U
25	1	2309	A
25	1	2310	C
25	1	2321	C
25	1	2333	A
25	1	2345	U
25	1	2350	C
25	1	2355	C
25	1	2356	A
25	1	2357	A
25	1	2359	G
25	1	2363	C
25	1	2368	G
25	1	2372	G
25	1	2394	G
25	1	2401	U
25	1	2404	C
25	1	2411	G
25	1	2423	A
25	1	2429	C
25	1	2433	G
25	1	2434	G
25	1	2466	C
25	1	2468	C
25	1	2494	G
25	1	2504	C
25	1	2506	C
25	1	2508	G
25	1	2509	G
25	1	2514	G
25	1	2515	G
25	1	2519	C

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Mol	Chain	Res	Type
25	1	2528	C
25	1	2530	G
25	1	2531	C
25	1	2537	A
25	1	2545	C
25	1	2546	C
25	1	2556	G
25	1	2557	G
25	1	2564	C
25	1	2568	C
25	1	2573	G
25	1	2574	C
25	1	2575	C
25	1	2580	C
25	1	2581	C
25	1	2582	C
25	1	2583	C
25	1	2584	G
25	1	2585	U
25	1	2587	C
25	1	2591	C
25	1	2592	U
25	1	2593	G
25	1	2594	C
25	1	2596	C
25	1	2598	A
25	1	2599	G
25	1	2600	G
25	1	2608	C
25	1	2609	G
25	1	2614	G
25	1	2627	G
25	1	2628	C
25	1	2646	C
25	1	2652	G
25	1	2672	G
25	1	2678	C
25	1	2683	C
25	1	2688	A
25	1	2690	G
25	1	2691	C
25	1	2692	G

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Mol	Chain	Res	Type
26	3	13	C
26	3	19	G
26	3	23	A
26	3	37	G
26	3	38	U
26	3	39	U
26	3	54	G
26	3	65	A
26	3	73	C
26	3	77	U
26	3	101	A
26	3	107	G
26	3	108	G
26	3	111	G
26	3	115	A
26	3	117	C
27	42	7	C
27	42	9	C
27	42	12	C
27	42	13	G
27	42	24	C
27	42	30	G
27	42	33	C
27	42	35	G
27	42	36	C
27	42	40	G
27	42	49	G
27	42	51	C
27	42	52	G
27	42	60	A
27	42	63	C
27	42	64	G
27	42	69	G
27	42	73	A
27	42	74	C
27	42	76	C
27	42	79	C
27	42	80	C
27	42	86	G
27	42	87	A
27	42	100	C
27	42	104	A

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Mol	Chain	Res	Type
27	42	105	A
27	42	106	C
27	42	109	A
27	42	112	G
27	42	114	G
27	42	115	C
27	42	119	G
27	42	120	G
27	42	122	G
66	w2	2	G
66	w2	69	C
66	w2	70	G
66	w2	76	A
68	E	76	A
73	2	3	U
73	2	4	C
73	2	9	C
73	2	17	C
73	2	26	G
73	2	33	U
73	2	40	G
73	2	41	G
73	2	44	G
73	2	45	A
73	2	46	A
73	2	54	A
73	2	56	G
73	2	64	A
73	2	71	A
73	2	87	A2M
73	2	91	C
73	2	92	A
73	2	101	A
73	2	116	C
73	2	125	C
73	2	129	A
73	2	130	C
73	2	134	G
73	2	137	G
73	2	142	C
73	2	152	A
73	2	153	G

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Mol	Chain	Res	Type
73	2	154	A
73	2	155	C
73	2	158	G
73	2	161	C
73	2	162	G
73	2	170	G
73	2	171	G
73	2	172	G
73	2	173	C
73	2	176	C
73	2	177	C
73	2	186	G
73	2	193	G
73	2	198	A
73	2	202	A
73	2	203	C
73	2	204	G
73	2	205	G
73	2	214	G
73	2	223	G
73	2	228	C
73	2	229	A
73	2	230	C
73	2	234	G
73	2	241	C
73	2	245	C
73	2	249	G
73	2	250	C
73	2	263	C
73	2	264	G
73	2	271	G
73	2	272	G
73	2	273	C
73	2	282	A
73	2	289	G
73	2	290	A
73	2	292	U
73	2	302	G
73	2	308	G
73	2	312	G
73	2	313	A
73	2	314	C

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Mol	Chain	Res	Type
73	2	316	G
73	2	324	A
73	2	329	A
73	2	330	G
73	2	335	G
73	2	336	C
73	2	337	A
73	2	338	G
73	2	340	A
73	2	351	U
73	2	353	G
73	2	356	C
73	2	357	A
73	2	363	C
73	2	365	G
73	2	366	C
73	2	378	C
73	2	387	G
73	2	389	G
73	2	390	C
73	2	391	G
73	2	394	A
73	2	396	U
73	2	400	G
73	2	406	C
73	2	427	G
73	2	432	G
73	2	438	G
73	2	446	C
73	2	449	G
73	2	454	C
73	2	455	G
73	2	458	G
73	2	459	U
73	2	460	A
73	2	461	A
73	2	464	C
73	2	475	A
73	2	476	G
73	2	477	C
73	2	491	G
73	2	500	G

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Mol	Chain	Res	Type
73	2	501	A
73	2	503	A
73	2	504	C
73	2	506	C
73	2	519	C
73	2	520	C
73	2	521	C
73	2	527	C
73	2	534	G
73	2	540	G
73	2	545	G
73	2	546	C
73	2	554	A
73	2	555	G
73	2	562	U
73	2	566	C
73	2	569	G
73	2	570	C
73	2	578	G
73	2	579	A
73	2	582	G
73	2	588	C
73	2	589	G
73	2	594	C
73	2	595	G
73	2	600	G
73	2	601	C
73	2	602	C
73	2	603	G
73	2	604	C
73	2	605	G
73	2	606	G
73	2	608	A
73	2	614	G
73	2	615	A
73	2	625	G
73	2	628	G
73	2	629	G
73	2	633	A
73	2	650	A
73	2	651	C
73	2	659	A

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Mol	Chain	Res	Type
73	2	662	G
73	2	665	U
73	2	685	G
73	2	687	C
73	2	704	A
73	2	711	C
73	2	712	U
73	2	718	A
73	2	722	A
73	2	740	C
73	2	744	A
73	2	756	C
73	2	757	A
73	2	759	C
73	2	778	A
73	2	780	C
73	2	784	G
73	2	791	C
73	2	792	G
73	2	794	G
73	2	804	C
73	2	812	G
73	2	833	G
73	2	834	G
73	2	836	G
73	2	839	U
73	2	840	C
73	2	842	G
73	2	850	G
73	2	851	G
73	2	856	G
73	2	868	OMG
73	2	880	A
73	2	888	G
73	2	892	G
73	2	900	C
73	2	903	C
73	2	909	G
73	2	921	G
73	2	927	U
73	2	928	C
73	2	932	C

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Mol	Chain	Res	Type
73	2	934	C
73	2	936	A
73	2	938	G
73	2	942	G
73	2	943	C
73	2	984	C
73	2	1009	U
73	2	1010	G
73	2	1011	OMG
73	2	1014	C
73	2	1018	G
73	2	1022	C
73	2	1025	C
73	2	1027	A
73	2	1028	G
73	2	1041	G
73	2	1054	U
73	2	1055	U
73	2	1056	G
73	2	1057	C
73	2	1059	A
73	2	1061	A
73	2	1076	G
73	2	1080	G
73	2	1088	C
73	2	1089	G
73	2	1090	C
73	2	1096	G
73	2	1099	C
73	2	1102	C
73	2	1112	A
73	2	1119	C
73	2	1125	G
73	2	1126	A
73	2	1129	G
73	2	1131	A
73	2	1132	G
73	2	1139	G
73	2	1140	A
73	2	1146	U
73	2	1147	C
73	2	1160	C

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Mol	Chain	Res	Type
73	2	1162	G
73	2	1163	C
73	2	1167	C
73	2	1175	A
73	2	1190	C
73	2	1191	G
73	2	1192	G
73	2	1194	G
73	2	1196	C
73	2	1197	C
73	2	1200	G
73	2	1203	G
73	2	1204	A
73	2	1208	G
73	2	1225	G
73	2	1226	C
73	2	1227	C
73	2	1230	G
73	2	1236	G
73	2	1242	G
73	2	1244	A
73	2	1245	C
73	2	1254	G
73	2	1257	C
73	2	1261	7MG
73	2	1262	A
73	2	1269	U
73	2	1270	G
73	2	1280	G
73	2	1282	C
73	2	1283	C
73	2	1287	C
73	2	1293	G
73	2	1295	C
73	2	1305	C
73	2	1320	C
73	2	1321	A
73	2	1343	U
73	2	1344	G
73	2	1351	G
73	2	1356	G
73	2	1366	G

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Mol	Chain	Res	Type
73	2	1367	A
73	2	1374	A
73	2	1381	G
73	2	1384	A
73	2	1388	C
73	2	1389	C
73	2	1391	G
73	2	1393	G
73	2	1394	C
73	2	1406	A
73	2	1408	A
73	2	1409	A
73	2	1410	G
73	2	1413	G
73	2	1419	A
73	2	1422	U
73	2	1433	G
73	2	1436	C
73	2	1445	G
73	2	1446	G
73	2	1447	A
73	2	1448	U
73	2	1449	C
73	2	1452	U

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	1	218	G
25	1	325	A
25	1	348	A
25	1	492	G
25	1	573	G
25	1	576	G
25	1	589	C
25	1	632	G
25	1	675	C
25	1	790	G
25	1	807	G
25	1	1204	OMG
25	1	1247	G
25	1	1381	C

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Mol	Chain	Res	Type
25	1	1477	C
25	1	1487	C
25	1	1587	G
25	1	1860	A
25	1	1871	C
25	1	1905	G
25	1	2354	U
25	1	2530	G
25	1	2536	A
25	1	2595	C
26	3	38	U
26	3	107	G
27	42	103	G
27	42	114	G
73	2	8	U
73	2	204	G
73	2	329	A
73	2	365	G
73	2	589	G
73	2	593	C
73	2	596	G
73	2	600	G
73	2	603	G
73	2	835	A
73	2	850	G
73	2	941	C
73	2	1009	U
73	2	1118	G
73	2	1199	C
73	2	1203	G
73	2	1380	C

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

40 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
73	OMC	2	104	73	19,22,23	0.85	0	26,31,34	0.99	1 (3%)
25	OMG	1	1520	25	18,26,27	1.02	1 (5%)	19,38,41	1.20	3 (15%)
25	OMG	1	1882	25,75	18,26,27	1.02	1 (5%)	19,38,41	1.37	3 (15%)
73	MA6	2	1435	73	18,26,27	1.02	1 (5%)	19,38,41	3.68	2 (10%)
73	7MG	2	1261	73	22,26,27	3.75	10 (45%)	29,39,42	2.09	9 (31%)
25	OMG	1	1204	25	18,26,27	2.34	7 (38%)	19,38,41	1.86	7 (36%)
25	OMG	1	1775	25	18,26,27	2.30	8 (44%)	19,38,41	1.46	3 (15%)
25	OMG	1	2074	25	18,26,27	2.30	7 (38%)	19,38,41	1.41	3 (15%)
25	A2M	1	1768	25	18,25,26	3.64	8 (44%)	18,36,39	3.47	6 (33%)
25	OMU	1	1897	25,75	19,22,23	2.90	7 (36%)	26,31,34	1.77	4 (15%)
25	OMC	1	2380	25	19,22,23	2.82	8 (42%)	26,31,34	0.89	1 (3%)
73	A2M	2	87	73,75	18,25,26	3.66	7 (38%)	18,36,39	3.28	4 (22%)
73	OMU	2	1314	73	19,22,23	2.90	8 (42%)	26,31,34	1.74	5 (19%)
27	OMG	42	133	27,25	18,26,27	2.34	8 (44%)	19,38,41	1.36	4 (21%)
25	A2M	1	396	25,75	18,25,26	0.95	1 (5%)	18,36,39	1.27	2 (11%)
73	M7A	2	1390	73	20,25,26	0.42	0	28,37,40	0.69	1 (3%)
25	A2M	1	393	25	18,25,26	3.56	8 (44%)	18,36,39	3.24	4 (22%)
25	OMC	1	1824	25	19,22,23	0.79	0	26,31,34	1.19	1 (3%)
73	A2M	2	348	76,73	18,25,26	3.62	8 (44%)	18,36,39	3.39	3 (16%)
25	OMG	1	313	25	18,26,27	2.33	8 (44%)	19,38,41	1.51	3 (15%)
25	OMG	1	2237	25,75	18,26,27	1.05	1 (5%)	19,38,41	1.06	2 (10%)
73	OMG	2	371	73	18,26,27	1.08	1 (5%)	19,38,41	1.35	3 (15%)
25	OMU	1	1896	25,75	19,22,23	2.89	8 (42%)	26,31,34	1.75	5 (19%)
25	OMU	1	49	25,75	19,22,23	2.94	7 (36%)	26,31,34	1.71	6 (23%)
25	A2M	1	523	25	18,25,26	3.54	8 (44%)	18,36,39	3.47	4 (22%)
25	OMG	1	624	25,75	18,26,27	2.33	7 (38%)	19,38,41	1.70	5 (26%)
73	4AC	2	1426	73,75	21,24,25	4.44	16 (76%)	29,34,37	1.37	3 (10%)
73	MA6	2	1434	73	18,26,27	1.04	1 (5%)	19,38,41	3.44	2 (10%)
25	OMC	1	1684	25,75	19,22,23	2.75	7 (36%)	26,31,34	0.97	1 (3%)
73	OMG	2	1035	73,75	18,26,27	2.44	8 (44%)	19,38,41	1.64	4 (21%)
25	OMU	1	1908	25	19,22,23	4.24	15 (78%)	26,31,34	1.92	7 (26%)
73	OMG	2	868	73	18,26,27	2.35	8 (44%)	19,38,41	1.40	2 (10%)
25	5MC	1	1765	25	18,22,23	3.26	7 (38%)	26,32,35	1.10	3 (11%)
25	OMG	1	1121	25	18,26,27	1.04	1 (5%)	19,38,41	1.45	3 (15%)
25	5MC	1	2292	25,75	18,22,23	3.36	7 (38%)	26,32,35	1.29	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
73	OMG	2	1011	73	18,26,27	1.00	1 (5%)	19,38,41	1.18	3 (15%)
73	C4J	2	933	73	24,29,30	3.35	9 (37%)	29,42,45	1.35	4 (13%)
25	OMG	1	386	25	18,26,27	0.98	1 (5%)	19,38,41	1.12	3 (15%)
25	OMG	1	2042	25,68	18,26,27	2.33	8 (44%)	19,38,41	1.41	3 (15%)
73	4OC	2	1325	73	20,23,24	3.04	8 (40%)	26,32,35	0.96	1 (3%)

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
73	OMC	2	104	73	-	1/9/27/28	0/2/2/2
25	OMG	1	1520	25	-	1/5/27/28	0/3/3/3
25	OMG	1	1882	25,75	-	0/5/27/28	0/3/3/3
73	MA6	2	1435	73	-	3/7/29/30	0/3/3/3
73	7MG	2	1261	73	-	0/7/37/38	0/3/3/3
25	OMG	1	1204	25	-	0/5/27/28	0/3/3/3
25	OMG	1	1775	25	-	2/5/27/28	0/3/3/3
25	OMG	1	2074	25	-	1/5/27/28	0/3/3/3
25	A2M	1	1768	25	-	2/5/27/28	0/3/3/3
25	OMU	1	1897	25,75	-	0/9/27/28	0/2/2/2
25	OMC	1	2380	25	-	0/9/27/28	0/2/2/2
73	A2M	2	87	73,75	-	3/5/27/28	0/3/3/3
73	OMU	2	1314	73	-	0/9/27/28	0/2/2/2
27	OMG	42	133	27,25	-	0/5/27/28	0/3/3/3
25	A2M	1	396	25,75	-	1/5/27/28	0/3/3/3
73	M7A	2	1390	73	-	2/7/37/38	0/3/3/3
25	A2M	1	393	25	-	0/5/27/28	0/3/3/3
25	OMC	1	1824	25	-	1/9/27/28	0/2/2/2
73	A2M	2	348	76,73	-	0/5/27/28	0/3/3/3
25	OMG	1	313	25	-	2/5/27/28	0/3/3/3
25	OMG	1	2237	25,75	-	0/5/27/28	0/3/3/3
73	OMG	2	371	73	-	1/5/27/28	0/3/3/3
25	OMU	1	1896	25,75	-	0/9/27/28	0/2/2/2
25	OMU	1	49	25,75	-	1/9/27/28	0/2/2/2
25	A2M	1	523	25	-	1/5/27/28	0/3/3/3
25	OMG	1	624	25,75	-	1/5/27/28	0/3/3/3
73	4AC	2	1426	73,75	-	2/11/29/30	0/2/2/2
73	MA6	2	1434	73	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	OMC	1	1684	25,75	-	4/9/27/28	0/2/2/2
73	OMG	2	1035	73,75	-	1/5/27/28	0/3/3/3
25	OMU	1	1908	25	-	2/9/27/28	0/2/2/2
73	OMG	2	868	73	-	3/5/27/28	0/3/3/3
25	5MC	1	1765	25	-	0/7/25/26	0/2/2/2
25	OMG	1	1121	25	-	2/5/27/28	0/3/3/3
25	5MC	1	2292	25,75	-	4/7/25/26	0/2/2/2
73	OMG	2	1011	73	-	1/5/27/28	0/3/3/3
73	C4J	2	933	73	-	6/16/34/35	0/2/2/2
25	OMG	1	386	25	-	0/5/27/28	0/3/3/3
25	OMG	1	2042	25,68	-	0/5/27/28	0/3/3/3
73	4OC	2	1325	73	-	0/9/29/30	0/2/2/2

All (235) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	2	933	C4J	C6-C5	12.11	1.52	1.34
25	1	1908	OMU	C3'-C2'	-10.39	1.29	1.52
25	1	2292	5MC	C6-C5	8.97	1.49	1.34
25	1	523	A2M	C3'-C4'	-8.76	1.30	1.53
73	2	87	A2M	C3'-C4'	-8.73	1.30	1.53
73	2	1426	4AC	O4'-C1'	8.71	1.62	1.42
25	1	393	A2M	C3'-C4'	-8.68	1.30	1.53
73	2	1261	7MG	C8-N9	8.64	1.50	1.46
25	1	1765	5MC	C6-C5	8.56	1.48	1.34
73	2	348	A2M	C3'-C4'	-8.42	1.31	1.53
25	1	1768	A2M	C3'-C4'	-8.40	1.31	1.53
73	2	87	A2M	O4'-C4'	8.05	1.63	1.45
25	1	1768	A2M	O4'-C1'	-7.76	1.30	1.41
73	2	1261	7MG	C5-N7	7.71	1.44	1.35
73	2	348	A2M	O4'-C4'	7.66	1.62	1.45
73	2	348	A2M	O4'-C1'	-7.55	1.30	1.41
25	1	393	A2M	O4'-C4'	7.49	1.61	1.45
25	1	1768	A2M	O4'-C4'	7.36	1.61	1.45
25	1	523	A2M	O4'-C1'	-7.36	1.30	1.41
73	2	87	A2M	O4'-C1'	-7.13	1.31	1.41
25	1	523	A2M	O4'-C4'	7.10	1.60	1.45
25	1	393	A2M	O4'-C1'	-7.10	1.31	1.41
25	1	1896	OMU	C2-N1	7.05	1.49	1.38
25	1	1897	OMU	C2-N1	6.93	1.49	1.38
73	2	1426	4AC	C4-N3	6.90	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	2	1426	4AC	C2'-C1'	-6.79	1.31	1.53
25	1	49	OMU	C2-N1	6.75	1.49	1.38
73	2	1426	4AC	C6-C5	6.74	1.50	1.35
73	2	1325	4OC	C4-N3	6.69	1.44	1.32
73	2	1314	OMU	C2-N1	6.60	1.49	1.38
73	2	1314	OMU	C2-N3	6.49	1.49	1.38
25	1	1908	OMU	C2-N1	6.32	1.48	1.38
25	1	49	OMU	C2-N3	6.32	1.49	1.38
73	2	933	C4J	C2-N3	6.26	1.49	1.38
25	1	1896	OMU	C2-N3	6.14	1.48	1.38
73	2	1261	7MG	C2-N3	5.99	1.47	1.33
73	2	1325	4OC	C6-C5	5.97	1.48	1.35
25	1	2380	OMC	C6-C5	5.97	1.48	1.35
25	1	1897	OMU	C2-N3	5.96	1.48	1.38
73	2	1261	7MG	C4-N9	5.90	1.44	1.37
25	1	1908	OMU	C2-N3	5.71	1.48	1.38
73	2	1325	4OC	C2-N3	5.65	1.47	1.36
25	1	2380	OMC	C2-N3	5.60	1.47	1.36
73	2	1261	7MG	C4-N3	5.59	1.47	1.34
25	1	1684	OMC	C2-N3	5.59	1.47	1.36
25	1	1684	OMC	C6-C5	5.59	1.48	1.35
25	1	49	OMU	C6-C5	5.51	1.47	1.35
25	1	2292	5MC	C4-N3	5.39	1.43	1.34
25	1	1765	5MC	C4-N3	5.39	1.43	1.34
25	1	2042	OMG	C2-N3	5.35	1.46	1.33
25	1	1765	5MC	C2-N3	5.31	1.47	1.36
73	2	1035	OMG	C2-N3	5.30	1.46	1.33
27	42	133	OMG	C2-N3	5.29	1.46	1.33
73	2	1426	4AC	C2-N1	5.28	1.51	1.40
73	2	1314	OMU	C6-C5	5.28	1.47	1.35
25	1	624	OMG	C2-N3	5.27	1.46	1.33
25	1	1908	OMU	C6-C5	5.26	1.47	1.35
25	1	1896	OMU	C6-C5	5.23	1.47	1.35
25	1	1897	OMU	C6-C5	5.22	1.47	1.35
25	1	2292	5MC	C2-N3	5.18	1.46	1.36
25	1	1775	OMG	C2-N3	5.09	1.45	1.33
73	2	868	OMG	C2-N3	5.02	1.45	1.33
73	2	1261	7MG	C2-N2	4.98	1.46	1.34
73	2	1426	4AC	C2-N3	4.94	1.46	1.36
25	1	1204	OMG	C2-N3	4.88	1.45	1.33
73	2	1426	4AC	O4'-C4'	-4.86	1.34	1.45
25	1	313	OMG	C2-N3	4.83	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	2	1426	4AC	C7-N4	4.76	1.46	1.37
73	2	1325	4OC	C4-N4	4.69	1.45	1.35
25	1	2074	OMG	C2-N3	4.68	1.44	1.33
25	1	1908	OMU	O4'-C1'	-4.68	1.30	1.42
25	1	1908	OMU	O4'-C4'	4.67	1.55	1.45
25	1	1684	OMC	C4-N3	4.65	1.43	1.34
25	1	2042	OMG	C4-N3	4.62	1.48	1.37
25	1	2074	OMG	C4-N3	4.61	1.48	1.37
25	1	2380	OMC	C4-N4	4.58	1.44	1.33
25	1	624	OMG	C4-N3	4.48	1.48	1.37
25	1	2292	5MC	C6-N1	4.47	1.45	1.38
27	42	133	OMG	C4-N3	4.47	1.48	1.37
73	2	1035	OMG	C4-N3	4.41	1.48	1.37
25	1	313	OMG	C4-N3	4.40	1.48	1.37
73	2	1426	4AC	C4-N4	4.38	1.46	1.39
25	1	1775	OMG	C4-N3	4.31	1.47	1.37
25	1	2380	OMC	C4-N3	4.29	1.43	1.34
25	1	1684	OMC	C4-N4	4.24	1.43	1.33
73	2	868	OMG	C4-N3	4.20	1.47	1.37
25	1	2380	OMC	C2-N1	4.18	1.49	1.40
25	1	1204	OMG	C4-N3	4.16	1.47	1.37
25	1	1765	5MC	C6-N1	4.09	1.45	1.38
73	2	868	OMG	C2-N2	4.09	1.43	1.34
25	1	2292	5MC	C2-N1	4.06	1.48	1.40
25	1	1908	OMU	O4-C4	-4.03	1.16	1.24
73	2	1261	7MG	C2-N1	3.95	1.47	1.37
73	2	1325	4OC	C2-N1	3.94	1.48	1.40
25	1	1684	OMC	C2-N1	3.94	1.48	1.40
73	2	1426	4AC	C5-C4	3.94	1.49	1.40
73	2	1035	OMG	C2-N2	3.87	1.43	1.34
73	2	933	C4J	C6-N1	3.86	1.46	1.36
73	2	1314	OMU	C4-N3	3.85	1.45	1.38
25	1	1765	5MC	C4-N4	3.80	1.44	1.34
25	1	1768	A2M	O3'-C3'	3.78	1.51	1.43
25	1	1204	OMG	C2-N2	3.75	1.43	1.34
73	2	933	C4J	C2-N1	3.75	1.50	1.39
25	1	1775	OMG	C2-N2	3.74	1.43	1.34
25	1	2042	OMG	C2-N2	3.73	1.43	1.34
27	42	133	OMG	C2-N2	3.72	1.43	1.34
25	1	1908	OMU	C2'-C1'	3.71	1.62	1.53
73	2	1426	4AC	O3'-C3'	-3.69	1.34	1.43
25	1	2292	5MC	C4-N4	3.69	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	1765	5MC	C2-N1	3.69	1.48	1.40
25	1	1897	OMU	C4-N3	3.67	1.45	1.38
73	2	933	C4J	C1'-C5	-3.67	1.41	1.50
25	1	1765	5MC	O2-C2	-3.66	1.16	1.23
25	1	2292	5MC	O2-C2	-3.64	1.17	1.23
73	2	1035	OMG	C6-N1	3.64	1.43	1.37
25	1	49	OMU	O4-C4	-3.61	1.17	1.24
25	1	1896	OMU	O4-C4	-3.58	1.17	1.24
25	1	1897	OMU	O4-C4	-3.54	1.17	1.24
25	1	1908	OMU	C5'-C4'	-3.53	1.40	1.51
25	1	624	OMG	C2-N2	3.51	1.42	1.34
25	1	1684	OMC	O2-C2	-3.48	1.17	1.23
73	2	1325	4OC	C5-C4	3.48	1.48	1.40
73	2	1261	7MG	C5-C6	3.47	1.52	1.43
73	2	1426	4AC	CM7-C7	3.45	1.57	1.50
25	1	49	OMU	C4-N3	3.43	1.44	1.38
25	1	313	OMG	C2-N2	3.41	1.42	1.34
25	1	2074	OMG	C2-N2	3.38	1.42	1.34
73	2	1325	4OC	O2-C2	-3.36	1.17	1.23
25	1	313	OMG	O6-C6	-3.31	1.16	1.23
73	2	933	C4J	C4-N3	3.28	1.46	1.40
25	1	1204	OMG	C6-N1	3.27	1.42	1.37
73	2	1314	OMU	O4-C4	-3.25	1.18	1.24
25	1	1908	OMU	O2-C2	-3.23	1.17	1.23
27	42	133	OMG	C6-N1	3.22	1.42	1.37
73	2	868	OMG	O6-C6	-3.21	1.16	1.23
25	1	49	OMU	O2-C2	-3.21	1.17	1.23
25	1	1897	OMU	O2-C2	-3.21	1.17	1.23
25	1	1896	OMU	C4-N3	3.18	1.44	1.38
73	2	348	A2M	O3'-C3'	3.17	1.50	1.43
25	1	2380	OMC	O2-C2	-3.14	1.17	1.23
25	1	2074	OMG	C6-N1	3.14	1.42	1.37
25	1	2380	OMC	C6-N1	3.12	1.45	1.38
73	2	1325	4OC	C6-N1	3.11	1.45	1.38
73	2	1426	4AC	O5'-C5'	-3.11	1.37	1.44
73	2	933	C4J	O4-C4	-3.10	1.16	1.23
25	1	2074	OMG	O6-C6	-3.09	1.17	1.23
25	1	1908	OMU	C4-N3	3.09	1.44	1.38
25	1	1204	OMG	C5-C4	-3.08	1.35	1.43
73	2	868	OMG	C6-N1	3.06	1.42	1.37
25	1	2237	OMG	C6-N1	-3.06	1.33	1.37
73	2	1035	OMG	C5-C4	-3.03	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	2	348	A2M	C6-N6	3.03	1.45	1.34
25	1	1684	OMC	C6-N1	3.02	1.45	1.38
25	1	1768	A2M	C5-C4	-3.02	1.33	1.40
73	2	1261	7MG	C6-N1	3.00	1.44	1.38
25	1	523	A2M	C6-N6	2.99	1.45	1.34
25	1	313	OMG	C5-C4	-2.99	1.35	1.43
73	2	87	A2M	C6-N6	2.99	1.45	1.34
25	1	313	OMG	C6-N1	2.96	1.42	1.37
25	1	1775	OMG	O6-C6	-2.94	1.17	1.23
25	1	624	OMG	C6-N1	2.93	1.42	1.37
73	2	87	A2M	O3'-C3'	2.88	1.49	1.43
73	2	1426	4AC	O2'-C2'	2.88	1.49	1.43
73	2	1035	OMG	O6-C6	-2.88	1.17	1.23
25	1	624	OMG	C5-C4	-2.87	1.35	1.43
25	1	1204	OMG	O6-C6	-2.87	1.17	1.23
25	1	393	A2M	C5-C4	-2.86	1.33	1.40
25	1	1882	OMG	C6-N1	-2.86	1.33	1.37
25	1	2042	OMG	O6-C6	-2.86	1.17	1.23
73	2	1434	MA6	C5-C4	-2.85	1.33	1.40
25	1	2074	OMG	C5-C4	-2.85	1.35	1.43
25	1	523	A2M	O3'-C3'	2.85	1.49	1.43
73	2	933	C4J	O4'-C1'	-2.84	1.39	1.43
25	1	624	OMG	C5-C6	2.84	1.53	1.47
25	1	1775	OMG	C5-C4	-2.82	1.35	1.43
25	1	1896	OMU	O2-C2	-2.82	1.17	1.23
73	2	1426	4AC	O7-C7	-2.82	1.16	1.23
25	1	313	OMG	C5-C6	2.81	1.53	1.47
25	1	1204	OMG	C5-C6	2.80	1.53	1.47
73	2	87	A2M	C5-C4	-2.78	1.33	1.40
73	2	1435	MA6	C5-C4	-2.78	1.33	1.40
25	1	2074	OMG	C5-C6	2.77	1.53	1.47
25	1	393	A2M	O2'-C2'	-2.76	1.35	1.42
25	1	386	OMG	C6-N1	-2.75	1.33	1.37
25	1	1768	A2M	C6-N6	2.73	1.44	1.34
25	1	1520	OMG	C6-N1	-2.72	1.33	1.37
25	1	1908	OMU	C6-N1	2.72	1.44	1.38
73	2	1314	OMU	O2-C2	-2.72	1.18	1.23
73	2	1314	OMU	C6-N1	2.69	1.44	1.38
25	1	624	OMG	O6-C6	-2.69	1.17	1.23
25	1	2042	OMG	C5-C6	2.69	1.52	1.47
25	1	49	OMU	C6-N1	2.69	1.44	1.38
25	1	1121	OMG	C6-N1	-2.68	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	2	348	A2M	O2'-C2'	-2.68	1.35	1.42
25	1	1896	OMU	C6-N1	2.68	1.44	1.38
73	2	348	A2M	C5-C4	-2.67	1.33	1.40
25	1	393	A2M	C6-N6	2.66	1.43	1.34
27	42	133	OMG	O6-C6	-2.66	1.17	1.23
73	2	371	OMG	C6-N1	-2.65	1.33	1.37
73	2	868	OMG	C2-N1	2.65	1.44	1.37
25	1	1908	OMU	O5'-C5'	-2.65	1.38	1.44
73	2	1261	7MG	O6-C6	-2.62	1.18	1.23
25	1	1908	OMU	O3'-C3'	2.62	1.49	1.43
73	2	87	A2M	O2'-C2'	-2.61	1.35	1.42
27	42	133	OMG	C5-C4	-2.61	1.36	1.43
25	1	2042	OMG	C6-N1	2.61	1.41	1.37
73	2	1011	OMG	C6-N1	-2.59	1.34	1.37
25	1	1768	A2M	O2'-C2'	-2.57	1.36	1.42
25	1	523	A2M	O2'-C2'	-2.56	1.36	1.42
25	1	523	A2M	C5-C4	-2.55	1.34	1.40
25	1	2042	OMG	C5-C4	-2.53	1.36	1.43
25	1	1897	OMU	C6-N1	2.53	1.44	1.38
25	1	1775	OMG	C6-N1	2.51	1.41	1.37
73	2	1426	4AC	C6-N1	2.51	1.44	1.38
27	42	133	OMG	C5-C6	2.50	1.52	1.47
73	2	1035	OMG	C5-C6	2.48	1.52	1.47
25	1	393	A2M	O3'-C3'	2.47	1.48	1.43
25	1	396	A2M	C5-C4	2.41	1.47	1.40
73	2	868	OMG	C5-C4	-2.40	1.37	1.43
25	1	1775	OMG	C5-C6	2.38	1.52	1.47
73	2	933	C4J	O2-C2	-2.34	1.18	1.22
73	2	1035	OMG	C2-N1	2.33	1.43	1.37
25	1	2380	OMC	C5-C4	2.31	1.48	1.42
25	1	1775	OMG	C2-N1	2.31	1.43	1.37
25	1	313	OMG	C2-N1	2.29	1.43	1.37
73	2	868	OMG	C5-C6	2.24	1.52	1.47
27	42	133	OMG	C2-N1	2.20	1.43	1.37
25	1	1908	OMU	C5-C4	2.18	1.48	1.43
25	1	523	A2M	O5'-C5'	-2.13	1.39	1.44
25	1	1896	OMU	C5-C4	2.12	1.48	1.43
73	2	1314	OMU	C5-C4	2.10	1.48	1.43
25	1	1768	A2M	O5'-C5'	-2.06	1.39	1.44
73	2	348	A2M	C2-N3	2.05	1.35	1.32
25	1	2042	OMG	C2-N1	2.01	1.42	1.37
25	1	393	A2M	O5'-C5'	-2.01	1.39	1.44

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	2	1435	MA6	N1-C6-N6	-14.68	101.61	117.06
73	2	1434	MA6	N1-C6-N6	-13.78	102.55	117.06
25	1	523	A2M	C5-C6-N6	10.88	136.88	120.35
73	2	348	A2M	C5-C6-N6	10.56	136.40	120.35
73	2	87	A2M	C5-C6-N6	10.32	136.03	120.35
25	1	1768	A2M	C5-C6-N6	10.24	135.91	120.35
25	1	393	A2M	C5-C6-N6	9.77	135.21	120.35
25	1	1768	A2M	N6-C6-N1	-7.28	103.47	118.57
73	2	348	A2M	N6-C6-N1	-7.27	103.49	118.57
25	1	523	A2M	N6-C6-N1	-7.26	103.50	118.57
25	1	393	A2M	N6-C6-N1	-6.89	104.27	118.57
73	2	87	A2M	N6-C6-N1	-6.75	104.57	118.57
25	1	1768	A2M	N3-C2-N1	-5.69	119.79	128.68
25	1	523	A2M	N3-C2-N1	-5.51	120.07	128.68
73	2	1435	MA6	N3-C2-N1	-5.48	120.12	128.68
73	2	1314	OMU	C4-N3-C2	-5.44	119.40	126.58
25	1	1897	OMU	C4-N3-C2	-5.38	119.49	126.58
25	1	393	A2M	N3-C2-N1	-5.37	120.28	128.68
73	2	348	A2M	N3-C2-N1	-5.35	120.31	128.68
73	2	1434	MA6	N3-C2-N1	-5.23	120.50	128.68
73	2	1261	7MG	C5-C6-N1	5.20	120.16	110.99
73	2	87	A2M	N3-C2-N1	-5.11	120.69	128.68
25	1	1896	OMU	C4-N3-C2	-5.02	119.95	126.58
25	1	49	OMU	C4-N3-C2	-4.83	120.21	126.58
25	1	1908	OMU	C4-N3-C2	-4.70	120.38	126.58
73	2	1261	7MG	C2-N3-C4	4.64	120.56	112.30
25	1	49	OMU	N3-C2-N1	4.39	120.72	114.89
73	2	1261	7MG	C5-C4-N3	-4.27	119.99	128.13
25	1	1824	OMC	C2'-C1'-N1	-4.20	106.06	114.22
25	1	1908	OMU	N3-C2-N1	4.02	120.23	114.89
25	1	1896	OMU	N3-C2-N1	3.86	120.02	114.89
73	2	933	C4J	C4-N3-C2	-3.84	120.61	125.46
25	1	1897	OMU	N3-C2-N1	3.77	119.90	114.89
73	2	1314	OMU	C5-C4-N3	3.76	120.47	114.84
25	1	1897	OMU	C5-C4-N3	3.73	120.42	114.84
25	1	1896	OMU	C5-C4-N3	3.65	120.30	114.84
73	2	1035	OMG	C5-C6-N1	3.63	120.36	113.95
73	2	1314	OMU	N3-C2-N1	3.56	119.62	114.89
25	1	2292	5MC	C5-C6-N1	-3.55	119.68	123.34
25	1	1204	OMG	C5-C6-N1	3.49	120.11	113.95
25	1	1775	OMG	C5-C6-N1	3.38	119.92	113.95
25	1	313	OMG	C5-C6-N1	3.29	119.77	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	2042	OMG	C5-C6-N1	3.24	119.68	113.95
73	2	1035	OMG	C2-N1-C6	-3.24	119.13	125.10
73	2	868	OMG	C5-C6-N1	3.21	119.62	113.95
25	1	1897	OMU	O4-C4-C5	-3.18	119.57	125.16
25	1	2074	OMG	C5-C6-N1	3.17	119.55	113.95
25	1	624	OMG	C5-C6-N1	3.17	119.55	113.95
25	1	393	A2M	C1'-N9-C4	3.17	132.21	126.64
73	2	1314	OMU	O4-C4-C5	-3.15	119.63	125.16
25	1	396	A2M	N3-C2-N1	-3.12	123.80	128.68
25	1	1908	OMU	C5-C4-N3	3.09	119.47	114.84
25	1	1775	OMG	C2-N1-C6	-3.05	119.48	125.10
27	42	133	OMG	C5-C6-N1	3.04	119.32	113.95
73	2	1261	7MG	C4-C5-N7	3.02	109.72	105.53
25	1	1121	OMG	O2'-C2'-C1'	3.01	115.06	109.09
73	2	371	OMG	O2'-C2'-C1'	-3.01	103.13	109.09
73	2	1426	4AC	C5'-C4'-C3'	-3.01	103.92	115.18
73	2	87	A2M	C1'-N9-C4	2.99	131.90	126.64
25	1	624	OMG	C8-N7-C5	2.98	108.68	102.99
25	1	313	OMG	C8-N7-C5	2.98	108.67	102.99
25	1	1204	OMG	C8-N7-C5	2.94	108.60	102.99
25	1	1204	OMG	C2-N1-C6	-2.94	119.69	125.10
73	2	1261	7MG	N9-C4-N3	2.93	129.85	125.47
73	2	1261	7MG	C5-C4-N9	2.93	110.15	106.35
25	1	1882	OMG	C8-N7-C5	2.90	108.51	102.99
73	2	1035	OMG	C8-N7-C5	2.89	108.50	102.99
25	1	2042	OMG	C2-N1-C6	-2.87	119.81	125.10
73	2	1261	7MG	C2-N1-C6	-2.86	119.88	125.10
25	1	624	OMG	C2-N1-C6	-2.86	119.84	125.10
25	1	1765	5MC	C5-C6-N1	-2.85	120.41	123.34
25	1	49	OMU	C5-C4-N3	2.83	119.07	114.84
73	2	104	OMC	C2'-C1'-N1	-2.82	108.76	114.22
25	1	2074	OMG	C8-N7-C5	2.80	108.32	102.99
73	2	1261	7MG	O6-C6-C5	-2.76	120.76	127.54
25	1	1896	OMU	O4-C4-C5	-2.76	120.31	125.16
25	1	1204	OMG	O3'-C3'-C4'	2.75	119.00	111.05
25	1	624	OMG	O2'-C2'-C1'	2.74	114.53	109.09
25	1	396	A2M	C4-C5-N7	-2.71	106.57	109.40
25	1	1775	OMG	C8-N7-C5	2.71	108.15	102.99
25	1	2074	OMG	C2-N1-C6	-2.71	120.11	125.10
25	1	1908	OMU	O4'-C4'-C3'	-2.71	99.76	105.11
25	1	313	OMG	C2-N1-C6	-2.70	120.12	125.10
25	1	2042	OMG	C8-N7-C5	2.68	108.09	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	1204	OMG	O3'-C3'-C2'	2.67	118.75	111.17
25	1	386	OMG	C5-C6-N1	2.63	118.59	113.95
27	42	133	OMG	C2-N1-C6	-2.59	120.32	125.10
73	2	1426	4AC	O2-C2-N3	-2.58	118.14	122.33
25	1	1882	OMG	C5-C6-N1	2.56	118.48	113.95
73	2	1325	4OC	C6-C5-C4	2.55	120.08	116.96
25	1	1121	OMG	C8-N7-C5	2.52	107.78	102.99
25	1	1908	OMU	O4'-C4'-C5'	2.52	117.65	109.37
73	2	1011	OMG	C5-C6-N1	2.50	118.37	113.95
27	42	133	OMG	C8-N7-C5	2.50	107.75	102.99
25	1	1520	OMG	C5-C6-N1	2.48	118.34	113.95
25	1	1765	5MC	CM5-C5-C6	-2.48	119.53	122.85
73	2	868	OMG	C2-N1-C6	-2.48	120.53	125.10
25	1	2237	OMG	C8-N7-C5	2.42	107.60	102.99
25	1	1121	OMG	C5-C6-N1	2.41	118.21	113.95
25	1	49	OMU	O4-C4-C5	-2.41	120.93	125.16
25	1	1896	OMU	C1'-N1-C2	2.40	121.91	117.57
25	1	386	OMG	C8-N7-C5	2.39	107.54	102.99
25	1	1765	5MC	O2-C2-N3	-2.39	118.45	122.33
73	2	371	OMG	C5-C6-N1	2.39	118.16	113.95
73	2	1426	4AC	C5-C4-N3	-2.38	118.76	122.59
25	1	1520	OMG	C8-N7-C5	2.37	107.50	102.99
25	1	2237	OMG	C5-C6-N1	2.36	118.12	113.95
73	2	933	C4J	O35-C34-C32	2.35	121.38	113.38
25	1	2292	5MC	C1'-N1-C6	2.33	125.00	121.12
25	1	1768	A2M	O2'-C2'-C1'	2.31	113.68	109.09
73	2	1035	OMG	O6-C6-C5	-2.31	119.86	124.37
73	2	1011	OMG	C8-N7-C5	2.31	107.39	102.99
25	1	1908	OMU	O4'-C1'-N1	2.30	113.61	108.36
25	1	1768	A2M	O3'-C3'-C4'	2.29	117.67	111.05
25	1	2292	5MC	O2-C2-N3	-2.29	118.61	122.33
25	1	49	OMU	C6-N1-C2	-2.28	118.07	120.99
73	2	371	OMG	C8-N7-C5	2.27	107.31	102.99
73	2	1261	7MG	N9-C8-N7	2.24	106.59	103.38
73	2	933	C4J	C5-C4-N3	2.22	120.29	116.17
25	1	1882	OMG	C5'-C4'-C3'	-2.21	106.91	115.18
25	1	624	OMG	CM2-O2'-C2'	2.20	120.30	114.52
25	1	1768	A2M	O3'-C3'-C2'	2.20	117.41	111.17
25	1	1908	OMU	C5'-C4'-C3'	-2.17	107.03	115.18
25	1	2380	OMC	O2-C2-N3	-2.13	118.86	122.33
73	2	1314	OMU	O2-C2-N1	-2.12	119.97	122.79
27	42	133	OMG	O6-C6-C5	-2.10	120.27	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	2	933	C4J	N3-C2-N1	2.10	119.72	116.76
25	1	1520	OMG	O6-C6-C5	-2.08	120.31	124.37
25	1	1684	OMC	O2-C2-N3	-2.07	118.97	122.33
25	1	1204	OMG	C3’-C2’-C1’	-2.07	99.00	102.89
25	1	49	OMU	O2-C2-N1	-2.07	120.04	122.79
25	1	386	OMG	O6-C6-C5	-2.05	120.36	124.37
25	1	523	A2M	O2’-C2’-C1’	2.05	113.16	109.09
25	1	1204	OMG	N2-C2-N1	2.02	121.02	116.71
73	2	1390	M7A	C5-C4-N9	2.01	109.26	106.44
73	2	1011	OMG	O6-C6-C5	-2.01	120.46	124.37

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	1	49	OMU	C1’-C2’-O2’-CM2
25	1	313	OMG	O4’-C4’-C5’-O5’
25	1	396	A2M	C1’-C2’-O2’-CM’
25	1	523	A2M	C1’-C2’-O2’-CM’
25	1	624	OMG	C1’-C2’-O2’-CM2
25	1	1121	OMG	C1’-C2’-O2’-CM2
25	1	1520	OMG	C1’-C2’-O2’-CM2
25	1	1775	OMG	O4’-C4’-C5’-O5’
25	1	1824	OMC	C1’-C2’-O2’-CM2
25	1	1908	OMU	C3’-C4’-C5’-O5’
25	1	1908	OMU	O4’-C4’-C5’-O5’
73	2	87	A2M	C1’-C2’-O2’-CM’
73	2	104	OMC	C1’-C2’-O2’-CM2
73	2	371	OMG	C3’-C2’-O2’-CM2
73	2	868	OMG	C1’-C2’-O2’-CM2
73	2	933	C4J	C3’-C4’-C5’-O5’
73	2	933	C4J	C4’-C5’-O5’-P
73	2	1011	OMG	C1’-C2’-O2’-CM2
73	2	1435	MA6	O4’-C4’-C5’-O5’
25	1	313	OMG	C3’-C4’-C5’-O5’
25	1	1775	OMG	C3’-C4’-C5’-O5’
73	2	87	A2M	O4’-C4’-C5’-O5’
73	2	1435	MA6	C3’-C4’-C5’-O5’
25	1	1684	OMC	C2’-C1’-N1-C6
25	1	1768	A2M	C3’-C4’-C5’-O5’
73	2	87	A2M	C3’-C4’-C5’-O5’
73	2	933	C4J	O4’-C4’-C5’-O5’

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Mol	Chain	Res	Type	Atoms
25	1	1684	OMC	C2'-C1'-N1-C2
73	2	868	OMG	C3'-C4'-C5'-O5'
73	2	1426	4AC	C3'-C4'-C5'-O5'
25	1	1768	A2M	O4'-C4'-C5'-O5'
73	2	868	OMG	O4'-C4'-C5'-O5'
73	2	933	C4J	C3-C31-C32-N33
73	2	1426	4AC	O4'-C4'-C5'-O5'
25	1	1684	OMC	O4'-C1'-N1-C6
25	1	1684	OMC	O4'-C1'-N1-C2
73	2	933	C4J	C31-C32-C34-O35
73	2	933	C4J	C31-C32-C34-O36
25	1	2292	5MC	C2'-C1'-N1-C6
25	1	2292	5MC	O4'-C1'-N1-C6
25	1	2074	OMG	C3'-C2'-O2'-CM2
73	2	1390	M7A	C4'-C5'-O5'-P
73	2	1435	MA6	C4'-C5'-O5'-P
25	1	1121	OMG	C4'-C5'-O5'-P
25	1	2292	5MC	O4'-C4'-C5'-O5'
25	1	2292	5MC	O4'-C1'-N1-C2
73	2	1035	OMG	C1'-C2'-O2'-CM2
73	2	1390	M7A	C2'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 556 ligands modelled in this entry, 556 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
66	w2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w2	5:G	O3'	68:C	P	17.08

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13683. 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)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section was not generated.