



## Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 11:17 PM EST

PDB ID : 6O90  
EMDB ID : EMD-0660  
Title : Cryo-EM image reconstruction of the 70S Ribosome *Enterococcus faecalis* Class05  
Authors : Jogl, G.; Khayat, R.  
Deposited on : 2019-03-12  
Resolution : 3.49 Å (reported)  
Based on initial models : 4YBB, 5LI0

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

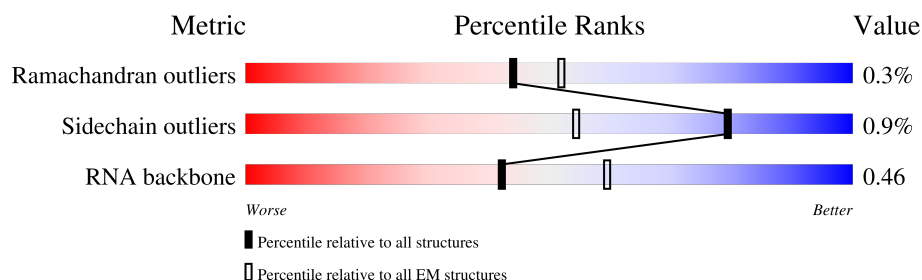
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.49 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.



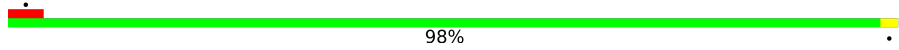
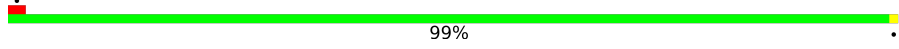
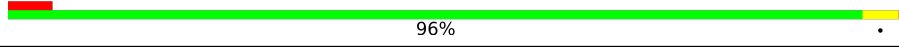
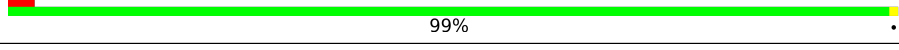
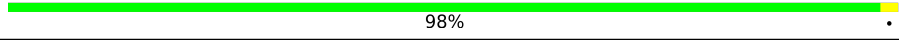
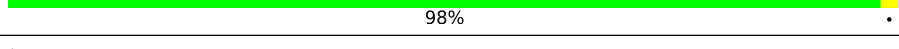
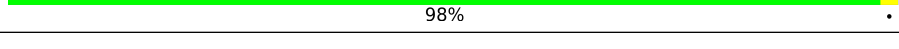
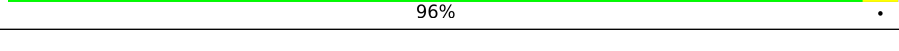
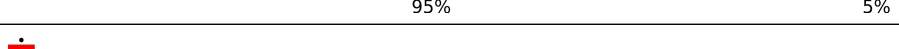
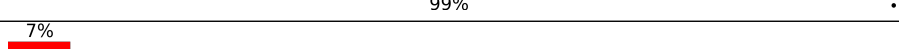
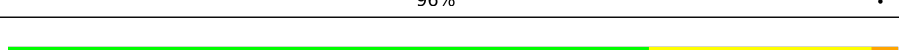

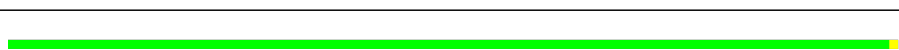
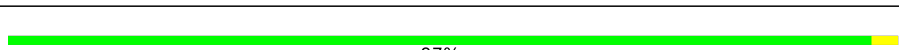
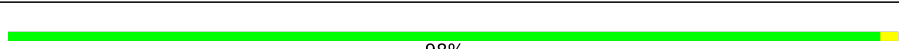
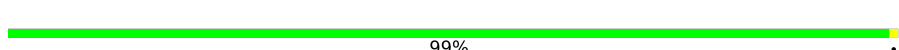
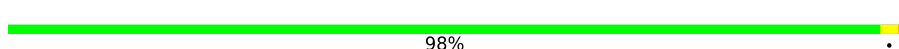
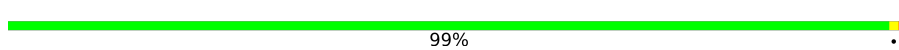
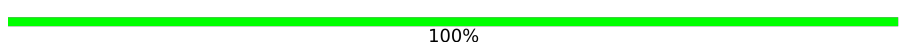
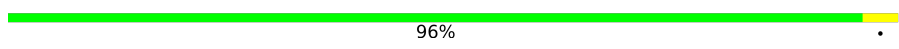
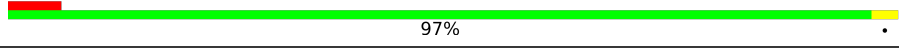
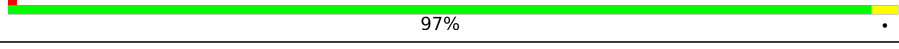
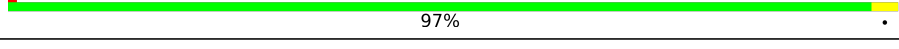
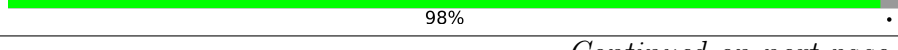

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	1528	
2	c	204	
3	d	201	
4	e	163	
5	f	97	
6	g	154	
7	h	131	
8	i	128	

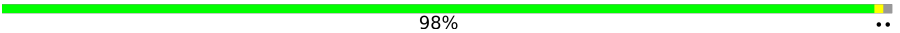
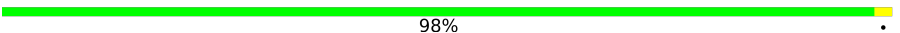
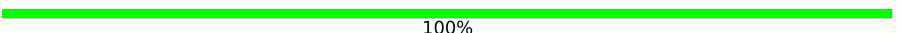
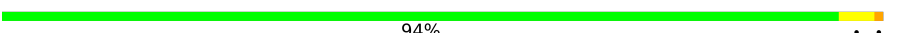
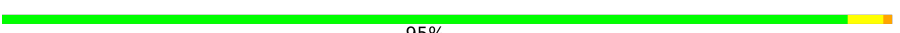





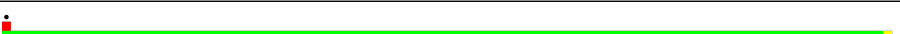


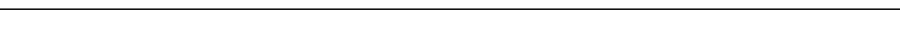
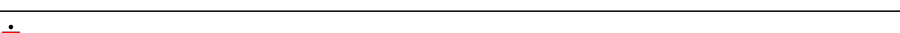
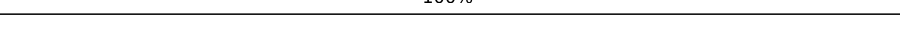
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Mol	Chain	Length	Quality of chain
9	j	99	 98%
10	k	117	 99%
11	l	136	 96%
12	m	112	 99%
13	n	60	 98%
14	o	88	 98%
15	p	89	 98%
16	q	83	 96%
17	r	66	 95% 5%
18	s	78	 99%
19	t	81	 96%
20	A	2903	 72% 25%
21	B	116	 72% 25%
22	C	275	 99%
23	D	207	 97%
24	E	206	 98%
25	F	177	 99%
26	G	176	 98%
27	K	145	 99%
28	L	122	 100%
29	M	146	 96%
30	N	141	 97%
31	O	123	 97%
32	P	117	 97%
33	Q	114	 98%

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Mol	Chain	Length	Quality of chain
34	R	118	 98% ..
35	S	102	 98% .
36	T	112	 100%
37	U	89	 94% . .
38	V	101	 95% . .
39	W	94	 65% 98% .
40	X	76	 97% .
41	Y	54	 94% 6%
42	Z	61	 98% .
43	0	58	 100%
44	1	83	 99% .
45	2	56	 100%
46	3	49	 100%
47	4	44	 98% .
48	5	64	 100%
49	6	38	 100%

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 138532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1528	Total	C	N	O	P	0	0
			32746	14609	5979	10630	1528		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	204	Total	C	N	O	S	0	0
			1610	1012	303	292	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	201	Total	C	N	O	S	0	0
			1620	1016	303	297	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	163	Total	C	N	O	S	0	0
			1204	759	222	221	2		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	97	Total	C	N	O	S	0	0
			795	501	137	154	3		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	154	Total	C	N	O	S	0	0
			1229	765	236	222	6		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			1041	662	184	193	2		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	128	Total	C	N	O	S	0	0
			990	615	197	177	1		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	99	Total	C	N	O	S	0	0
			800	504	147	147	2		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	117	Total	C	N	O	S	0	0
			863	533	165	161	4		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	136	Total	C	N	O	S	0	0
			1065	661	214	188	2		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	112	Total	C	N	O	S	0	0
			884	540	180	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	60	Total	C	N	O	S	0	0
			492	310	100	77	5		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	88	Total	C	N	O	S	0	0
			741	455	152	133	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	p	89	Total	C	N	O	S	0	0
			708	448	131	127	2		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	83	Total	C	N	O	S	0	0
			681	427	127	124	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	66	Total	C	N	O	S	0	0
			537	343	99	94	1		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	s	78	Total	C	N	O	S	0	0
			634	410	113	109	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	81	Total	C	N	O	S	0	0
			610	372	119	117	2		

- Molecule 20 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A	2903	Total	C	N	O	P	0	0
			62302	27811	11457	20131	2903		

- Molecule 21 is a RNA chain called 4S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	116	Total	C	N	O	P	0	0
			2478	1106	444	812	116		

- Molecule 22 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	275	Total	C	N	O	S	0	0
			2114	1310	416	381	7		

- Molecule 23 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	207	Total	C	N	O	S	0	0
			1577	992	292	289	4		

- Molecule 24 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	206	Total	C	N	O	S	0	0
			1573	984	290	297	2		

- Molecule 25 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	177	Total	C	N	O	S	0	0
			1391	887	239	259	6		

- Molecule 26 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	G	176	Total	C	N	O	S	0	0
			1344	842	243	255	4		

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	K	145	Total	C	N	O	S	0	0
			1129	713	205	207	4		

- Molecule 28 is a protein called 50S ribosomal protein L14.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	L	122	Total	C	N	O	S	0	0
			922	574	176	170	2		

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	M	146	Total	C	N	O	S	0	0
			1094	676	212	205	1		

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	141	Total	C	N	O	S	0	0
			1117	710	215	185	7		

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	O	123	Total	C	N	O	S	0	0
			978	602	190	183	3		

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	117	Total	C	N	O	S	0	0
			898	556	175	166	1		

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Q	112	Total	C	N	O	0	0
			897	566	177	154		

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R	117	Total	C	N	O	S	0	0
			940	597	181	158	4		

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S	102	Total	C	N	O	S	0	0
			783	499	139	143	2		

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	T	112	Total	C	N	O	S	0	0
			849	532	156	159	2		

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	U	89	Total	C	N	O	S	0	0
			719	457	127	132	3		

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	V	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	W	94	Total	C	N	O	S	0	0
			757	479	135	139	4		

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	X	76	Total	C	N	O	0	0
			571	351	108	112		

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Y	54	Total	C	N	O	S	0	0
			425	265	86	72	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Z	61	Total	C	N	O	S	0	0
			504	314	94	95	1		

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	0	58	Total	C	N	O	S	0	0
			434	270	81	82	1		

- Molecule 44 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	83	Total	C	N	O	S	0	0
			673	424	114	133	2		

- Molecule 45 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	56	Total	C	N	O	S	0	0
			429	262	88	73	6		

- Molecule 46 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	49	Total	C	N	O	S	0	0
			418	253	85	76	4		

- Molecule 47 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

- Molecule 48 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 49 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	6	38	Total	C	N	O	S	0	0
			303	188	66	43	6		

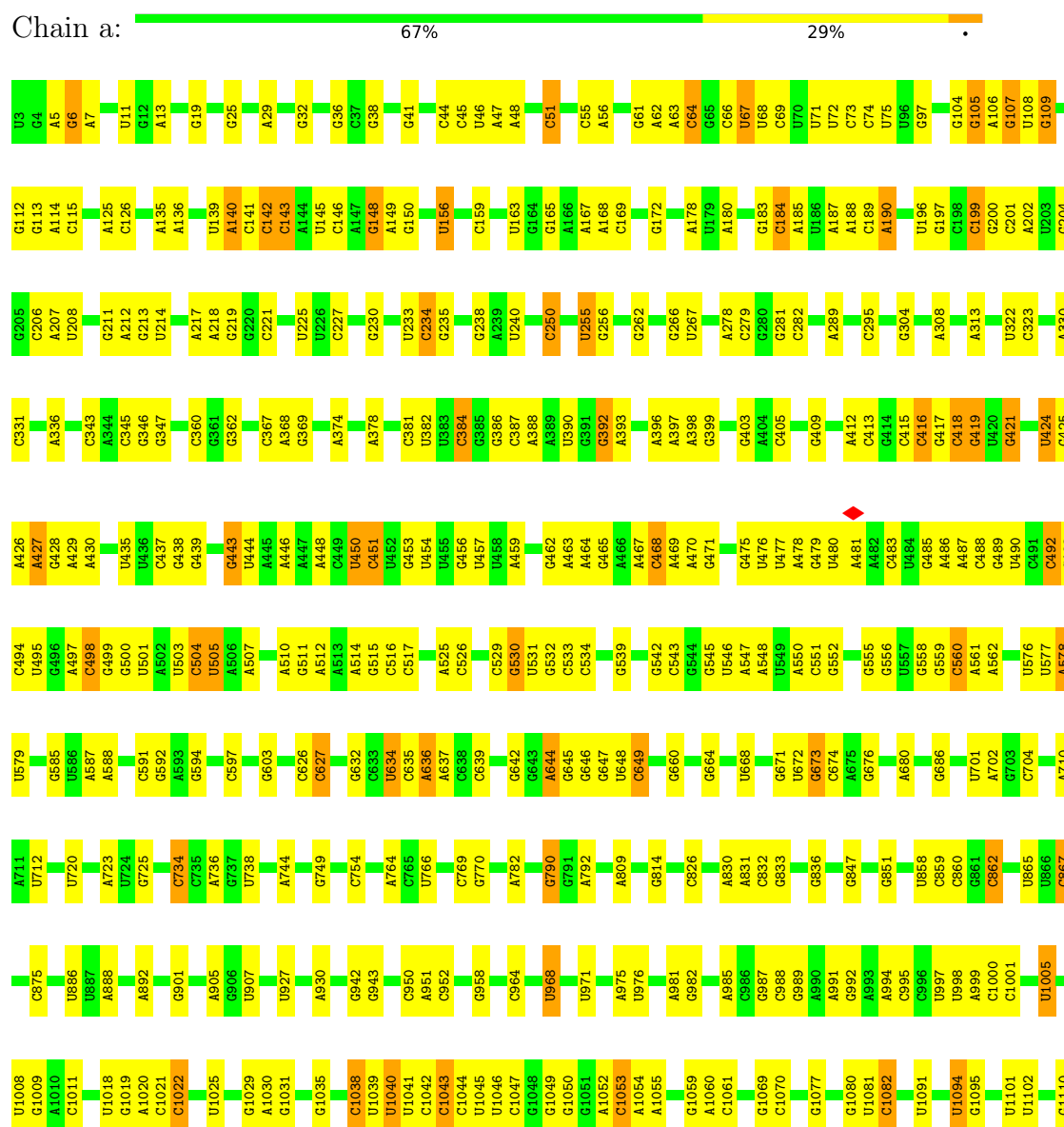
- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

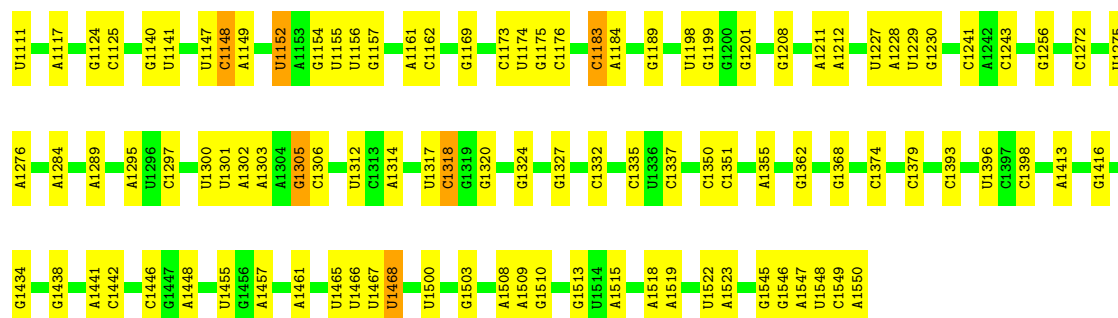
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			1	1	
50	2	1	Total	Zn	0
			1	1	
50	3	1	Total	Zn	0
			1	1	
50	6	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

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

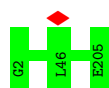
#### • Molecule 1: 16S rRNA





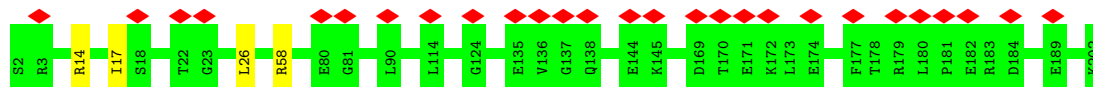
- Molecule 2: 30S ribosomal protein S3

Chain c:  100%



- Molecule 3: 30S ribosomal protein S4

Chain d:  13% 98%



- Molecule 4: 30S ribosomal protein S5

Chain e:  100%

There are no outlier residues recorded for this chain.

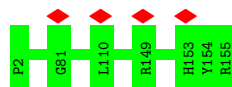
- Molecule 5: 30S ribosomal protein S6

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: 30S ribosomal protein S7

Chain g:  100%



- Molecule 7: 30S ribosomal protein S8

Chain h:  100%

There are no outlier residues recorded for this chain.

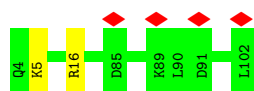
- Molecule 8: 30S ribosomal protein S9

Chain i:  98% .



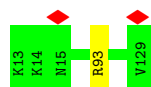
- Molecule 9: 30S ribosomal protein S10

Chain j:  98% .



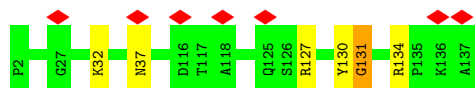
- Molecule 10: 30S ribosomal protein S11

Chain k:  99% .



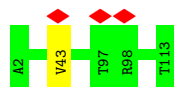
- Molecule 11: 30S ribosomal protein S12

Chain l:  5% 96% ..



- Molecule 12: 30S ribosomal protein S13

Chain m:  99% .



- Molecule 13: 30S ribosomal protein S14 type Z

Chain n:  98% .



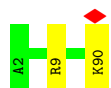
- Molecule 14: 30S ribosomal protein S15

Chain o:  98% .



- Molecule 15: 30S ribosomal protein S16

Chain p:  98%



- Molecule 16: 30S ribosomal protein S17

Chain q:  96%



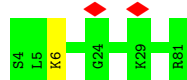
- Molecule 17: 30S ribosomal protein S18

Chain r:  95%



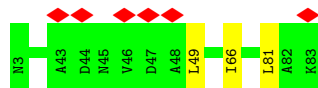
- Molecule 18: 30S ribosomal protein S19

Chain s:  99%



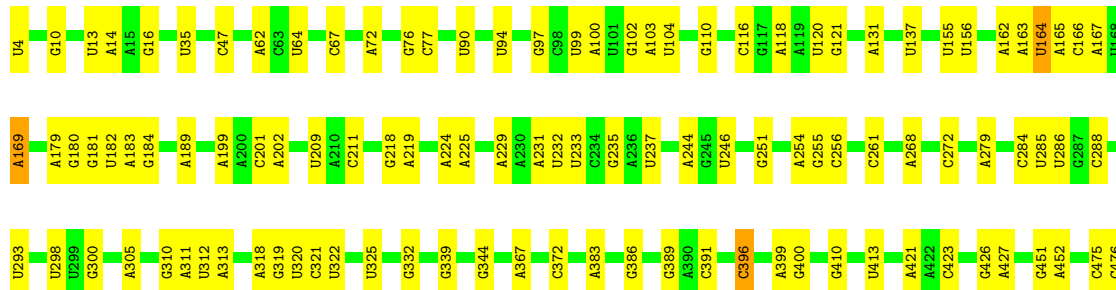
- Molecule 19: 30S ribosomal protein S20

Chain t:  7%



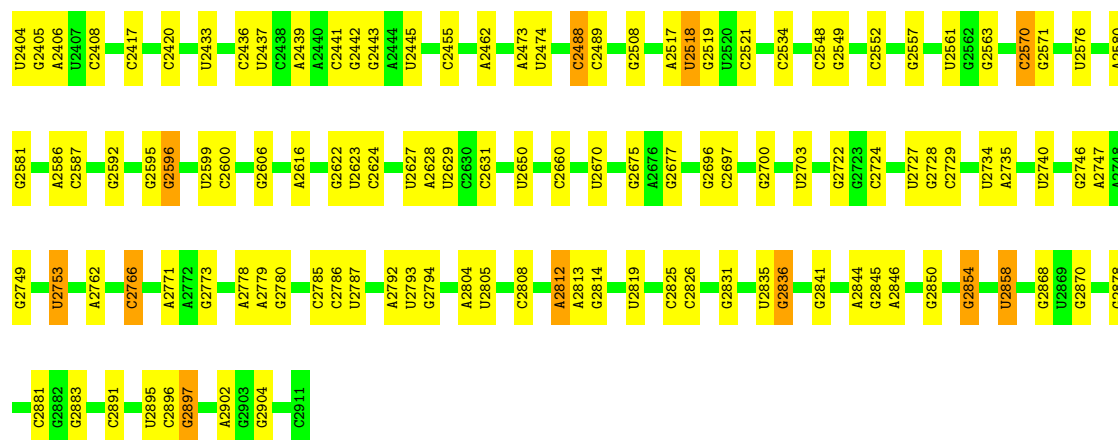
- Molecule 20: 23S rRNA

Chain A:  72%





C2262	G2139	G2006	U1841	U1877	G1568	U1365	A1182	A1110	A1014	G923	C778	C638	U488
C2278	A2140	U2007	G1842	C1689	G1569	C1366	A1188	G1111	A1015	C924	C779	G639	C495
C2280	G2141	C2010	A1843	G1690	G1573	C1369	U1189	C1112	G1016	C925	C780	A640	C496
A2281	C2142	G2020	G1853	C1691	G1574	C1375	U1190	C1114	A1023	C926	U787	U644	U499
A2282	G2144	U2021	G1872	C1699	G1575	U1376	G1197	C1115	G1024	U928	G788	C649	G507
G2293	A2145	U2030	U1878	C1703	A1576	U1377	A1209	C1116	G1029	C931	A792	G653	G508
G2296	G2147	G2035	C1882	C1717	U1577	U1378	A1212	C1117	C1034	G932	G805	A654	G509
C2297	A2148	U2036	G1885	C1718	U1579	G1470	U1215	C1118	G1035	G933	G808	A655	A517
A2301	G2154	A2037	U1886	A1719	U1581	G1471	A1216	C1119	A1036	U935	U824	A656	A518
A2302	G2158	C2038	G1886	U1723	A1586	C1479	G1217	C1120	C1046	G940	G815	A657	A519
C2307	U2160	G2039	G1886	C1737	G1589	G1395	U1218	C1121	C1047	A941	G816	G669	A520
C2311	A2045	A2044	A1896	A1741	G1601	A1396	G1219	U1122	A1048	U942	G817	A670	G521
C2317	G2162	G2046	G1902	C1746	U1602	C1400	C1234	C1126	C1049	U943	A822	G673	C527
G2318	U2163	A2047	C1906	G1768	C1603	A1401	C1238	G1127	A1050	U944	A823	A544	
U2319	G2173	U2048	C1907	C1769	A1604	G1404	G1249	U1128	U1052	C945	U824	A676	U547
G2176	G2174	G2049	A1913	C1751	C1605	U1496	G1257	G1129	A1053	A950	G832	U677	U548
A2323	G2175	C2050	G1917	G1770	A1606	U1497	U1275	U1130	G1057	A951	A833	C679	C549
C2327	G2179	G2062	G1920	C1757	U1608	U1408	G1276	U1134	C1057	A952	A834	U684	U550
A2333	U2181	G2066	A1927	C1758	A1612	G1411	C1277	A1135	A1061	C953	C835	U693	G559
A2334	G2182	C2069	G1928	C1768	A1613	U1421	U1287	U1136	G1062	C954	A840	U694	U560
G2335	U2183	G2070	G1936	C1770	G1614	C1422	C1288	U1137	U1063	C955	G845	A695	G561
A2336	A2187	A2074	G1943	A1776	C1623	U1428	G1289	C1140	G1065	U960	U847	G696	C566
G2337	C2188	G2075	G1944	G1777	U1627	C1431	U1289	U1141	A1066	C961	G848	A708	A567
U2340	G2196	A2076	C1948	C1784	G1628	U1432	C1293	C1142	U1073	C962	G849	G709	A568
A2341	A2201	C2077	A1952	A1782	A1630	C1433	U1296	C1144	G1074	A964	C852	C711	C569
G2348	C2206	U2082	A1955	C1783	A1631	U1434	C1304	U1145	U1075	U965	U867	C712	A571
A2349	C2207	G2083	C1955	G1784	A1632	C1435	U1308	G1146	C1085	U973	U885	A716	G572
A2350	C2208	U2090	U1969	A1787	A1634	U1436	A1309	U1147	G1086	A974	U886	G722	A585
C2361	A2212	U2114	U1970	G1790	C1638	U1439	A1310	C1149	G1087	U975	G887	U726	A586
C2364	A2213	G2115	G1978	U1795	C1641	A1439	A1311	C1150	C1092	G978	A888	C730	U587
G2367	G2217	C2121	A1980	C1798	C1642	G1443	G1317	C1151	U1093	A981	A891	G600	G588
A2372	C2218	U2125	C1981	C1802	C1646	U1446	U1336	G1152	G1096	G982	G893	C601	C602
G2379	A2224	A2126	A1984	C1814	U1650	U1447	U1337	A1167	U1098	U983	G900	G607	G607
A2390	A2225	C2127	A1985	A1815	U1651	U1448	U1338	A1168	A1097	A985	G901	G610	A611
G2393	U2227	G2130	G1986	A1823	A1652	U1450	U1339	U1170	G1102	C984	G897	A755	A612
C2397	A2239	U2132	G1989	A1829	C1653	U1451	U1349	C1171	C1104	A997	G907	A757	C821
G2398	C2240	A2133	U1990	A1830	G1654	U1452	C1350	A1172	U1105	A998	G909	A758	G622
C2399	G2252	G2134	U1996	G1831	C1655	U1454	A1357	C1174	U1106	A999	A919	G769	A623
	G2253	G2138	U2005	C1840	A1673	U1455	U1362	C1175	A1107	A1000	G920	A770	G629
					G1674	A1566	U1456	G1179	G1108	G1001	G921	A775	
						C1567	U1457	C1181	A1109	G1006	G922		



• Molecule 21: 4S rRNA

Chain B: 72% 25% .



• Molecule 22: 50S ribosomal protein L2

Chain C: 99% .



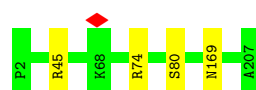
• Molecule 23: 50S ribosomal protein L3

Chain D: 97% .



• Molecule 24: 50S ribosomal protein L4

Chain E: 98% .



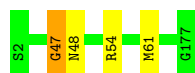
• Molecule 25: 50S ribosomal protein L5

Chain F: 99% .



• Molecule 26: 50S ribosomal protein L6

Chain G:  98% ..



- Molecule 27: 50S ribosomal protein L13

Chain K:  99% ..



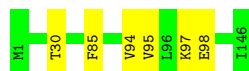
- Molecule 28: 50S ribosomal protein L14

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L15

Chain M:  96% .



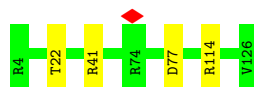
- Molecule 30: 50S ribosomal protein L16

Chain N:  6% 97% .



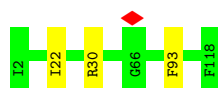
- Molecule 31: 50S ribosomal protein L17

Chain O:  97% .



- Molecule 32: 50S ribosomal protein L18

Chain P:  97% .



- Molecule 33: 50S ribosomal protein L19

Chain Q:  98% .



- Molecule 34: 50S ribosomal protein L20

Chain R:  98% ..



- Molecule 35: 50S ribosomal protein L21

Chain S:  98% .



- Molecule 36: 50S ribosomal protein L22

Chain T:  100%

There are no outlier residues recorded for this chain.

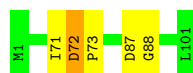
- Molecule 37: 50S ribosomal protein L23

Chain U:  94% ..



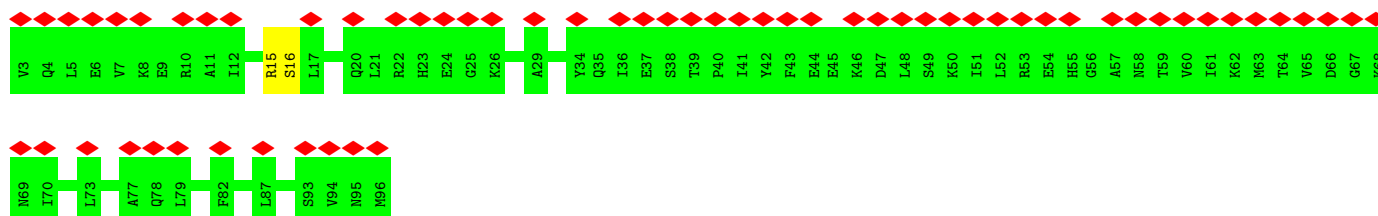
- Molecule 38: 50S ribosomal protein L24

Chain V:  95% ..



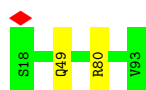
- Molecule 39: 50S ribosomal protein L25

Chain W:  65% 98% .



- Molecule 40: 50S ribosomal protein L27

Chain X:  97%



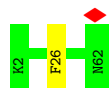
- Molecule 41: 50S ribosomal protein L28

Chain Y:  94%



- Molecule 42: 50S ribosomal protein L29

Chain Z:  98%



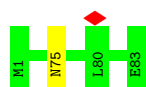
- Molecule 43: 50S ribosomal protein L30

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L31 type B

Chain 1:  99%



- Molecule 45: 50S ribosomal protein L32

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 50S ribosomal protein L33

Chain 3:  100%

There are no outlier residues recorded for this chain.

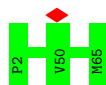
- Molecule 47: 50S ribosomal protein L34

Chain 4:  98%



- Molecule 48: 50S ribosomal protein L35

Chain 5:  100%



- Molecule 49: 50S ribosomal protein L36

Chain 6:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46244	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.323	Depositor
Minimum map value	-0.893	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.238	Depositor
Map size (Å)	482.68, 482.68, 482.68	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.097, 1.097, 1.097	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	a	0.65	2/36657 (0.0%)	1.19	299/57173 (0.5%)
2	c	0.31	0/1635	0.54	0/2197
3	d	0.33	0/1650	0.64	2/2217 (0.1%)
4	e	0.34	0/1217	0.62	0/1641
5	f	0.30	0/807	0.53	0/1087
6	g	0.29	0/1249	0.52	0/1682
7	h	0.36	0/1054	0.60	0/1417
8	i	0.32	0/1003	0.59	0/1343
9	j	0.30	0/812	0.65	0/1093
10	k	0.30	0/878	0.58	0/1185
11	l	0.38	0/1082	0.72	1/1453 (0.1%)
12	m	0.28	0/890	0.58	0/1195
13	n	0.33	0/504	0.53	0/669
14	o	0.33	0/751	0.57	0/1001
15	p	0.38	0/720	0.59	0/966
16	q	0.40	0/689	0.66	0/920
17	r	0.31	0/544	0.61	0/728
18	s	0.33	0/650	0.58	0/872
19	t	0.36	0/612	0.64	2/818 (0.2%)
20	A	0.89	3/69785 (0.0%)	1.20	461/108842 (0.4%)
21	B	0.72	1/2770 (0.0%)	1.17	17/4311 (0.4%)
22	C	0.50	0/2148	0.72	1/2888 (0.0%)
23	D	0.51	0/1597	0.72	0/2143
24	E	0.47	0/1595	0.63	0/2157
25	F	0.33	0/1410	0.59	0/1895
26	G	0.40	0/1362	0.67	1/1831 (0.1%)
27	K	0.50	0/1148	0.71	0/1546
28	L	0.51	0/929	0.66	0/1247
29	M	0.43	0/1102	0.78	0/1467
30	N	0.47	0/1139	0.73	0/1515
31	O	0.50	0/984	0.80	2/1317 (0.2%)
32	P	0.41	0/907	0.63	0/1214



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Q	0.51	0/911	0.67	0/1227
34	R	0.52	0/951	0.70	1/1260 (0.1%)
35	S	0.47	0/794	0.65	0/1064
36	T	0.46	0/858	0.66	0/1157
37	U	0.48	0/725	0.73	0/969
38	V	0.41	0/772	0.75	1/1035 (0.1%)
39	W	0.29	0/768	0.65	0/1032
40	X	0.54	0/576	0.70	0/768
41	Y	0.35	0/431	0.58	0/574
42	Z	0.39	0/505	0.59	0/672
43	0	0.42	0/434	0.67	0/583
44	1	0.33	0/690	0.62	0/930
45	2	0.56	0/436	0.70	0/578
46	3	0.38	0/422	0.57	0/561
47	4	0.48	0/377	0.65	0/491
48	5	0.43	0/528	0.66	0/689
49	6	0.51	0/308	0.62	0/407
All	All	0.73	6/150766 (0.0%)	1.09	788/226027 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	l	0	2
12	m	0	1
16	q	0	1
19	t	0	1
22	C	0	2
23	D	0	2
24	E	0	2
25	F	0	1
26	G	0	2
27	K	0	2
29	M	0	3
30	N	0	2
31	O	0	2
32	P	0	3
35	S	0	2
37	U	0	2
38	V	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
39	W	0	1
40	X	0	1
41	Y	0	1
47	4	0	1
All	All	0	36

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1	U	OP3-P	-10.56	1.48	1.61
20	A	1689	A	N9-C4	6.30	1.41	1.37
1	a	56	A	N9-C4	5.95	1.41	1.37
1	a	140	A	N9-C4	5.89	1.41	1.37
20	A	1288	A	N9-C4	-5.71	1.34	1.37
20	A	1414	A	N9-C4	-5.05	1.34	1.37

All (788) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	346	G	N7-C8-N9	11.73	118.96	113.10
20	A	1349	U	N3-C2-O2	-11.63	114.06	122.20
1	a	1548	U	N1-C2-O2	11.43	130.80	122.80
1	a	1082	C	N1-C2-O2	11.38	125.73	118.90
20	A	1551	U	C2-N1-C1'	11.38	131.36	117.70
20	A	1551	U	N1-C2-O2	11.22	130.65	122.80
20	A	644	U	N3-C2-O2	-10.82	114.63	122.20
1	a	1548	U	C2-N1-C1'	10.68	130.51	117.70
20	A	1130	U	N1-C2-O2	10.63	130.24	122.80
20	A	1130	U	C2-N1-C1'	10.49	130.29	117.70
1	a	109	G	O4'-C1'-N9	10.01	116.21	108.20
20	A	1551	U	N3-C2-O2	-9.99	115.21	122.20
20	A	1349	U	N1-C2-O2	9.90	129.73	122.80
1	a	1548	U	N3-C2-O2	-9.89	115.28	122.20
1	a	346	G	C8-N9-C4	-9.87	102.45	106.40
20	A	1130	U	N3-C2-O2	-9.71	115.40	122.20
1	a	1082	C	N3-C2-O2	-9.63	115.16	121.90
20	A	963	C	C6-N1-C2	-9.58	116.47	120.30
20	A	1106	U	N1-C2-O2	9.50	129.45	122.80
1	a	560	C	N1-C2-O2	9.49	124.59	118.90
1	a	826	C	C2-N1-C1'	9.43	129.17	118.80
1	a	579	U	N3-C2-O2	-9.38	115.63	122.20
1	a	1082	C	C2-N1-C1'	9.37	129.11	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	141	C	N1-C2-O2	9.37	124.52	118.90
1	a	142	C	N1-C2-O2	9.24	124.45	118.90
1	a	109	G	C8-N9-C1'	9.16	138.91	127.00
21	B	68	C	N1-C2-O2	9.16	124.40	118.90
1	a	346	G	C5-N7-C8	-9.15	99.72	104.30
21	B	68	C	C2-N1-C1'	9.15	128.87	118.80
20	A	644	U	N1-C2-O2	9.13	129.19	122.80
1	a	826	C	N1-C2-O2	9.06	124.34	118.90
20	A	901	U	C2-N1-C1'	9.05	128.56	117.70
20	A	1885	C	N1-C2-O2	9.03	124.32	118.90
20	A	2825	C	N1-C2-O2	9.01	124.31	118.90
1	a	108	U	N3-C2-O2	-8.99	115.91	122.20
20	A	1130	U	C5-C6-N1	8.96	127.18	122.70
1	a	1082	C	C6-N1-C2	-8.79	116.79	120.30
1	a	109	G	C4-N9-C1'	-8.73	115.15	126.50
1	a	56	A	C2-N3-C4	8.66	114.93	110.60
20	A	1489	C	C2-N3-C4	8.65	124.23	119.90
20	A	1349	U	C2-N1-C1'	8.62	128.05	117.70
1	a	492	C	N1-C2-O2	8.59	124.06	118.90
20	A	897	G	N3-C4-N9	-8.57	120.86	126.00
1	a	997	U	C2-N1-C1'	8.44	127.83	117.70
20	A	906	C	N1-C2-O2	8.43	123.96	118.90
20	A	849	G	N1-C6-O6	-8.40	114.86	119.90
1	a	579	U	N1-C2-O2	8.39	128.67	122.80
20	A	1148	U	N1-C2-O2	8.36	128.65	122.80
20	A	2825	C	N3-C2-O2	-8.36	116.05	121.90
20	A	1489	C	C5-C6-N1	8.33	125.17	121.00
20	A	1148	U	N3-C2-O2	-8.24	116.43	122.20
20	A	901	U	N1-C2-O2	8.22	128.55	122.80
1	a	1465	U	N1-C2-O2	8.19	128.53	122.80
20	A	1350	C	C2-N1-C1'	8.17	127.79	118.80
20	A	897	G	N9-C4-C5	8.17	108.67	105.40
1	a	468	C	C6-N1-C2	-8.15	117.04	120.30
20	A	261	C	N1-C2-O2	8.11	123.77	118.90
20	A	2697	C	N1-C2-O2	8.08	123.75	118.90
1	a	875	C	N1-C2-O2	8.06	123.73	118.90
1	a	505	U	C5-C6-N1	8.01	126.70	122.70
1	a	142	C	N3-C2-O2	-7.87	116.39	121.90
1	a	140	A	C2-N3-C4	7.87	114.53	110.60
20	A	1948	C	C2-N1-C1'	7.86	127.45	118.80
1	a	1173	C	C2-N1-C1'	7.84	127.43	118.80
1	a	826	C	C6-N1-C2	-7.79	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	730	C	C6-N1-C2	-7.79	117.19	120.30
20	A	1885	C	N3-C2-O2	-7.73	116.49	121.90
1	a	108	U	N1-C2-O2	7.71	128.19	122.80
1	a	141	C	N3-C2-O2	-7.70	116.51	121.90
1	a	1053	C	N1-C2-O2	7.69	123.51	118.90
1	a	826	C	N3-C2-O2	-7.68	116.53	121.90
1	a	109	G	N9-C4-C5	7.66	108.46	105.40
20	A	925	C	C2-N1-C1'	7.66	127.22	118.80
20	A	901	U	N3-C2-O2	-7.65	116.84	122.20
20	A	1758	C	C2-N1-C1'	7.60	127.16	118.80
20	A	1551	U	C6-N1-C1'	-7.59	110.58	121.20
1	a	1306	C	C2-N1-C1'	7.55	127.11	118.80
1	a	156	U	N1-C2-O2	7.53	128.07	122.80
1	a	184	C	N1-C2-O2	7.52	123.41	118.90
1	a	995	C	N1-C2-O2	7.52	123.41	118.90
20	A	2488	C	N1-C2-O2	7.51	123.41	118.90
20	A	2858	U	N3-C2-O2	-7.50	116.95	122.20
20	A	2753	U	N1-C2-O2	7.45	128.01	122.80
1	a	108	U	C5-C6-N1	7.44	126.42	122.70
20	A	2734	U	N3-C2-O2	-7.43	117.00	122.20
1	a	190	A	N7-C8-N9	7.42	117.51	113.80
1	a	579	U	C2-N1-C1'	7.42	126.61	117.70
20	A	549	C	N1-C2-O2	7.41	123.35	118.90
1	a	148	G	C2-N3-C4	7.41	115.60	111.90
1	a	1548	U	C6-N1-C1'	-7.38	110.87	121.20
20	A	1928	C	N1-C2-O2	7.38	123.33	118.90
20	A	1304	U	C2-N1-C1'	7.37	126.54	117.70
1	a	1059	G	N1-C6-O6	-7.36	115.48	119.90
1	a	1173	C	N1-C2-O2	7.36	123.32	118.90
1	a	632	G	N3-C4-N9	-7.36	121.58	126.00
20	A	1489	C	N1-C2-O2	7.36	123.32	118.90
20	A	2143	C	C5-C6-N1	7.36	124.68	121.00
20	A	1047	C	C6-N1-C2	-7.35	117.36	120.30
1	a	907	U	N1-C2-O2	7.34	127.94	122.80
20	A	2734	U	N1-C2-O2	7.34	127.94	122.80
20	A	246	U	N3-C2-O2	-7.33	117.07	122.20
1	a	790	G	N3-C4-N9	-7.33	121.61	126.00
1	a	109	G	C6-C5-N7	7.32	134.79	130.40
20	A	1497	U	N3-C2-O2	-7.31	117.08	122.20
1	a	1183	C	C2-N1-C1'	7.30	126.83	118.80
20	A	849	G	C5-C6-O6	7.30	132.98	128.60
1	a	1465	U	N3-C2-O2	-7.29	117.09	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	560	C	C2-N1-C1'	7.29	126.82	118.80
1	a	997	U	N3-C2-O2	-7.26	117.12	122.20
20	A	1885	C	C2-N1-C1'	7.26	126.78	118.80
1	a	234	C	N3-C2-O2	-7.25	116.83	121.90
20	A	2766	C	N1-C2-O2	7.25	123.25	118.90
1	a	860	C	N1-C2-O2	7.23	123.24	118.90
1	a	492	C	N3-C2-O2	-7.23	116.84	121.90
20	A	2143	C	C6-N1-C2	-7.22	117.41	120.30
20	A	654	A	C8-N9-C4	7.21	108.69	105.80
1	a	1152	U	N1-C2-O2	7.21	127.85	122.80
20	A	1350	C	C6-N1-C2	-7.21	117.42	120.30
1	a	529	C	C6-N1-C2	-7.20	117.42	120.30
20	A	2794	G	C4-N9-C1'	7.20	135.86	126.50
20	A	2753	U	N3-C2-O2	-7.19	117.17	122.20
1	a	64	C	C6-N1-C2	-7.17	117.43	120.30
1	a	279	C	C6-N1-C2	-7.17	117.43	120.30
1	a	907	U	N3-C2-O2	-7.16	117.19	122.20
20	A	272	C	C2-N1-C1'	7.16	126.68	118.80
20	A	1907	C	N3-C2-O2	-7.15	116.89	121.90
20	A	261	C	N3-C2-O2	-7.13	116.91	121.90
1	a	1053	C	N3-C2-O2	-7.13	116.91	121.90
1	a	66	C	C6-N1-C2	-7.12	117.45	120.30
20	A	272	C	C6-N1-C2	-7.12	117.45	120.30
21	B	68	C	N3-C2-O2	-7.11	116.92	121.90
20	A	935	U	N1-C2-O2	7.11	127.77	122.80
20	A	1907	C	N1-C2-O2	7.10	123.16	118.90
20	A	906	C	C2-N1-C1'	7.08	126.59	118.80
20	A	2858	U	N1-C2-O2	7.08	127.76	122.80
1	a	1152	U	C2-N1-C1'	7.07	126.19	117.70
1	a	67	U	C2-N1-C1'	7.04	126.14	117.70
1	a	115	C	N1-C2-O2	7.03	123.12	118.90
20	A	655	G	C8-N9-C4	7.03	109.21	106.40
1	a	451	C	N1-C2-O2	7.02	123.11	118.90
1	a	148	G	N3-C4-C5	-7.01	125.09	128.60
20	A	2697	C	N3-C2-O2	-7.01	117.00	121.90
1	a	468	C	N3-C2-O2	-7.00	117.00	121.90
20	A	246	U	N1-C2-O2	7.00	127.70	122.80
20	A	527	C	N1-C2-O2	7.00	123.10	118.90
1	a	196	U	N3-C2-O2	-7.00	117.30	122.20
20	A	935	U	C2-N1-C1'	6.99	126.09	117.70
1	a	1152	U	N3-C2-O2	-6.97	117.32	122.20
20	A	1604	A	P-O3'-C3'	6.96	128.06	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	504	C	N3-C2-O2	-6.96	117.03	121.90
20	A	1106	U	N3-C2-O2	-6.95	117.34	122.20
20	A	935	U	N3-C2-O2	-6.93	117.35	122.20
20	A	1689	A	C2-N3-C4	6.91	114.06	110.60
1	a	1059	G	C5-C6-O6	6.91	132.75	128.60
20	A	1157	C	C2-N1-C1'	6.90	126.39	118.80
1	a	1305	G	C4-N9-C1'	6.90	135.47	126.50
21	B	68	C	C6-N1-C1'	-6.89	112.53	120.80
1	a	995	C	C2-N1-C1'	6.87	126.35	118.80
20	A	1130	U	C6-N1-C2	-6.85	116.89	121.00
20	A	1574	C	N1-C2-O2	6.84	123.01	118.90
20	A	649	C	C5-C6-N1	6.81	124.41	121.00
1	a	418	C	N1-C2-O2	6.81	122.98	118.90
1	a	109	G	C4-C5-N7	-6.80	108.08	110.80
1	a	141	C	C6-N1-C2	-6.80	117.58	120.30
38	V	71	ILE	C-N-CA	6.79	138.68	121.70
1	a	450	U	C5-C6-N1	6.78	126.09	122.70
1	a	1022	C	N1-C2-O2	6.78	122.97	118.90
20	A	1641	C	C6-N1-C2	-6.78	117.59	120.30
1	a	649	C	C6-N1-C2	-6.78	117.59	120.30
20	A	1024	G	N3-C4-C5	-6.78	125.21	128.60
1	a	109	G	N3-C4-N9	-6.77	121.94	126.00
1	a	1038	C	N1-C2-O2	6.76	122.96	118.90
1	a	1082	C	C5-C6-N1	6.76	124.38	121.00
20	A	396	C	C2-N1-C1'	6.75	126.22	118.80
20	A	1948	C	N1-C2-O2	6.73	122.94	118.90
20	A	925	C	N1-C2-O2	6.73	122.94	118.90
1	a	1001	C	C2-N1-C1'	6.72	126.20	118.80
20	A	1148	U	C2-N1-C1'	6.72	125.77	117.70
20	A	1758	C	C6-N1-C2	-6.68	117.63	120.30
1	a	108	U	C6-N1-C2	-6.66	117.00	121.00
20	A	956	C	N1-C2-O2	6.66	122.89	118.90
20	A	2007	U	N3-C2-O2	-6.65	117.54	122.20
1	a	115	C	N3-C2-O2	-6.64	117.25	121.90
1	a	1173	C	N3-C2-O2	-6.63	117.26	121.90
20	A	963	C	N3-C2-O2	-6.63	117.26	121.90
20	A	1454	U	N3-C2-O2	-6.63	117.56	122.20
20	A	1197	G	N3-C4-N9	6.63	129.98	126.00
20	A	1217	G	O5'-P-OP1	-6.63	99.73	105.70
20	A	2729	C	C5-C6-N1	6.62	124.31	121.00
1	a	416	C	N1-C2-O2	6.62	122.87	118.90
21	B	35	C	C6-N1-C2	-6.61	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	527	C	N3-C2-O2	-6.61	117.28	121.90
20	A	1304	U	N1-C2-O2	6.60	127.42	122.80
1	a	511	G	C4-N9-C1'	6.60	135.08	126.50
1	a	140	A	N3-C4-N9	6.58	132.66	127.40
20	A	1024	G	N3-C4-N9	6.57	129.94	126.00
1	a	511	G	N3-C4-N9	6.57	129.94	126.00
20	A	2570	C	N1-C2-O2	6.57	122.84	118.90
1	a	418	C	C2-N1-C1'	6.56	126.02	118.80
1	a	1305	G	N3-C4-N9	6.56	129.94	126.00
20	A	1647	C	C6-N1-C2	-6.56	117.68	120.30
1	a	860	C	C2-N1-C1'	6.55	126.00	118.80
21	B	96	G	C4-N9-C1'	6.54	135.01	126.50
1	a	734	C	C2-N1-C1'	6.50	125.95	118.80
1	a	952	C	N1-C2-O2	6.50	122.80	118.90
1	a	734	C	N3-C2-O2	-6.49	117.36	121.90
20	A	2090	U	N1-C2-O2	6.49	127.34	122.80
1	a	578	A	C4-N9-C1'	6.48	137.97	126.30
1	a	1306	C	C6-N1-C2	-6.48	117.71	120.30
20	A	1561	U	C2-N1-C1'	6.48	125.47	117.70
20	A	931	C	C2-N1-C1'	6.48	125.93	118.80
20	A	906	C	N3-C2-O2	-6.46	117.38	121.90
20	A	1641	C	N1-C2-O2	6.46	122.77	118.90
20	A	1605	C	P-O3'-C3'	6.44	127.43	119.70
1	a	1094	U	N3-C2-O2	-6.43	117.70	122.20
20	A	310	G	C4-N9-C1'	6.43	134.85	126.50
1	a	55	C	C6-N1-C2	-6.41	117.74	120.30
1	a	1091	U	N3-C2-O2	-6.41	117.72	122.20
1	a	67	U	N1-C2-O2	6.40	127.28	122.80
20	A	1434	C	C2-N1-C1'	6.39	125.83	118.80
1	a	1306	C	C5-C6-N1	6.39	124.20	121.00
1	a	443	G	OP1-P-O3'	6.39	119.25	105.20
20	A	1882	C	C2-N1-C1'	6.39	125.83	118.80
1	a	649	C	N1-C2-O2	6.39	122.73	118.90
20	A	1970	U	N3-C2-O2	-6.39	117.73	122.20
1	a	1468	U	N1-C2-O2	6.37	127.26	122.80
1	a	184	C	N3-C2-O2	-6.37	117.44	121.90
1	a	511	G	C8-N9-C1'	-6.36	118.73	127.00
20	A	2819	U	N1-C2-O2	6.36	127.25	122.80
26	G	54	ARG	NE-CZ-NH1	-6.36	117.12	120.30
20	A	1212	A	C2-N3-C4	6.36	113.78	110.60
1	a	1039	U	C2-N1-C1'	6.36	125.33	117.70
20	A	549	C	C2-N1-C1'	6.35	125.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	504	C	C6-N1-C2	-6.35	117.76	120.30
20	A	2240	C	N1-C2-O2	6.34	122.71	118.90
20	A	104	U	N1-C2-O2	6.34	127.24	122.80
20	A	509	G	O4'-C1'-N9	6.34	113.27	108.20
1	a	1043	C	C6-N1-C2	-6.34	117.77	120.30
1	a	503	U	C5-C6-N1	6.33	125.87	122.70
1	a	997	U	N1-C2-O2	6.33	127.23	122.80
20	A	1885	C	C6-N1-C2	-6.33	117.77	120.30
20	A	2127	C	C2-N1-C1'	6.33	125.76	118.80
1	a	156	U	N3-C2-O2	-6.33	117.77	122.20
20	A	1584	G	P-O3'-C3'	6.33	127.29	119.70
20	A	1092	C	N1-C2-O2	6.32	122.69	118.90
20	A	2819	U	N3-C2-O2	-6.32	117.77	122.20
1	a	267	U	C2-N1-C1'	6.32	125.28	117.70
1	a	875	C	N3-C2-O2	-6.32	117.48	121.90
20	A	256	C	C6-N1-C2	-6.32	117.77	120.30
20	A	1369	C	N3-C2-O2	-6.32	117.48	121.90
20	A	1304	U	N3-C2-O2	-6.31	117.78	122.20
20	A	2881	C	C6-N1-C2	-6.31	117.78	120.30
20	A	1703	C	C6-N1-C2	-6.30	117.78	120.30
20	A	2307	C	C5-C6-N1	6.28	124.14	121.00
1	a	56	A	N3-C4-C5	-6.28	122.41	126.80
20	A	1156	C	C2-N1-C1'	6.27	125.70	118.80
1	a	1173	C	C6-N1-C2	-6.25	117.80	120.30
20	A	1024	G	C4-N9-C1'	6.24	134.62	126.50
20	A	423	C	N1-C2-O2	6.24	122.64	118.90
1	a	450	U	C2-N1-C1'	6.23	125.18	117.70
1	a	968	U	N3-C2-O2	-6.22	117.85	122.20
1	a	529	C	C5-C6-N1	6.20	124.10	121.00
20	A	2786	C	C6-N1-C2	-6.20	117.82	120.30
1	a	597	C	N1-C2-O2	6.19	122.62	118.90
20	A	1448	U	C2-N1-C1'	6.19	125.13	117.70
20	A	1130	U	C6-N1-C1'	-6.19	112.54	121.20
20	A	1435	C	N1-C2-O2	6.18	122.61	118.90
1	a	1125	C	N1-C2-O2	6.18	122.61	118.90
20	A	2488	C	C2-N1-C1'	6.18	125.60	118.80
20	A	602	C	C6-N1-C2	-6.18	117.83	120.30
20	A	1454	U	N1-C2-O2	6.17	127.12	122.80
20	A	901	U	C5-C6-N1	6.17	125.79	122.70
20	A	1238	C	C6-N1-C2	-6.17	117.83	120.30
20	A	2729	C	C6-N1-C2	-6.17	117.83	120.30
1	a	1091	U	C2-N1-C1'	6.16	125.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	826	C	C6-N1-C1'	-6.15	113.42	120.80
20	A	1641	C	C2-N1-C1'	6.15	125.56	118.80
20	A	2794	G	C8-N9-C1'	-6.15	119.01	127.00
20	A	1197	G	C4-N9-C1'	6.14	134.48	126.50
1	a	451	C	C5-C6-N1	6.14	124.07	121.00
20	A	1551	U	C5-C6-N1	6.14	125.77	122.70
1	a	255	U	O4'-C1'-N1	6.13	113.11	108.20
1	a	530	G	C4-N9-C1'	6.13	134.47	126.50
20	A	956	C	C2-N1-C1'	6.13	125.54	118.80
20	A	413	U	N3-C2-O2	-6.13	117.91	122.20
1	a	1318	C	C2-N1-C1'	6.12	125.53	118.80
20	A	1641	C	N3-C2-O2	-6.12	117.61	121.90
1	a	734	C	C6-N1-C2	-6.12	117.85	120.30
1	a	649	C	C2-N1-C1'	6.12	125.53	118.80
20	A	607	G	N3-C4-C5	-6.11	125.54	128.60
20	A	897	G	N1-C6-O6	-6.11	116.23	119.90
20	A	164	U	N1-C2-N3	6.10	118.56	114.90
20	A	310	G	N3-C4-N9	6.10	129.66	126.00
1	a	634	U	C2-N1-C1'	6.10	125.02	117.70
1	a	1305	G	C8-N9-C1'	-6.09	119.08	127.00
20	A	1399	C	C2-N1-C1'	6.09	125.50	118.80
1	a	140	A	N3-C4-C5	-6.08	122.54	126.80
20	A	709	G	C4-N9-C1'	6.07	134.40	126.50
20	A	47	C	C6-N1-C2	-6.07	117.87	120.30
20	A	2670	U	C2-N1-C1'	6.07	124.98	117.70
1	a	704	C	C6-N1-C2	-6.07	117.87	120.30
20	A	201	C	C2-N1-C1'	6.06	125.47	118.80
20	A	960	U	N3-C2-O2	-6.06	117.96	122.20
21	B	85	U	C5-C6-N1	6.05	125.73	122.70
1	a	468	C	N1-C2-O2	6.05	122.53	118.90
20	A	849	G	N9-C4-C5	6.05	107.82	105.40
1	a	142	C	C2-N1-C1'	6.05	125.45	118.80
1	a	322	U	N3-C2-O2	-6.04	117.97	122.20
1	a	1053	C	C6-N1-C2	-6.04	117.88	120.30
20	A	104	U	N3-C2-O2	-6.04	117.97	122.20
20	A	1497	U	N1-C2-O2	6.03	127.02	122.80
20	A	897	G	C5-C6-O6	6.02	132.22	128.60
1	a	995	C	N3-C2-O2	-6.02	117.68	121.90
20	A	209	U	N3-C2-O2	-6.02	117.99	122.20
20	A	1379	G	N3-C4-N9	6.02	129.61	126.00
20	A	1928	C	N3-C2-O2	-6.02	117.69	121.90
20	A	1970	U	N1-C2-O2	6.02	127.01	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	423	C	C2-N1-C1'	6.01	125.41	118.80
1	a	196	U	N1-C2-O2	6.00	127.00	122.80
20	A	2766	C	N3-C2-O2	-6.00	117.70	121.90
20	A	1830	A	N7-C8-N9	6.00	116.80	113.80
31	O	41	ARG	CA-CB-CG	5.99	126.59	113.40
20	A	924	C	C6-N1-C2	-5.99	117.90	120.30
20	A	1830	A	C8-N9-C4	-5.99	103.40	105.80
20	A	621	C	C5-C6-N1	5.98	123.99	121.00
1	a	865	U	N3-C2-O2	-5.98	118.02	122.20
1	a	1305	G	N3-C4-C5	-5.97	125.61	128.60
20	A	2766	C	C2-N1-C1'	5.97	125.36	118.80
1	a	649	C	N3-C2-O2	-5.97	117.72	121.90
1	a	143	C	N3-C2-O2	-5.96	117.73	121.90
20	A	325	U	N1-C2-O2	5.96	126.97	122.80
20	A	1574	C	N3-C2-O2	-5.96	117.73	121.90
20	A	1379	G	C4-N9-C1'	5.95	134.24	126.50
20	A	1489	C	C6-N1-C2	-5.95	117.92	120.30
20	A	256	C	C5-C6-N1	5.95	123.98	121.00
20	A	973	U	N3-C2-O2	-5.95	118.04	122.20
20	A	246	U	C2-N1-C1'	5.95	124.84	117.70
20	A	1453	U	C2-N1-C1'	5.95	124.83	117.70
20	A	272	C	N3-C2-O2	-5.94	117.74	121.90
1	a	1468	U	N3-C2-O2	-5.94	118.04	122.20
20	A	1758	C	N3-C2-O2	-5.94	117.74	121.90
20	A	602	C	N1-C2-O2	5.93	122.46	118.90
20	A	1830	A	C2-N3-C4	5.93	113.56	110.60
20	A	2826	C	C2-N1-C1'	5.93	125.32	118.80
1	a	279	C	C2-N1-C1'	5.92	125.32	118.80
20	A	1655	C	C6-N1-C2	-5.91	117.93	120.30
20	A	1197	G	C8-N9-C1'	-5.91	119.32	127.00
20	A	2127	C	N1-C2-O2	5.90	122.44	118.90
20	A	1081	U	N3-C2-O2	-5.90	118.07	122.20
1	a	632	G	N9-C4-C5	5.89	107.76	105.40
1	a	560	C	C6-N1-C1'	-5.89	113.73	120.80
20	A	712	C	C6-N1-C2	-5.89	117.94	120.30
20	A	925	C	C6-N1-C2	-5.89	117.95	120.30
20	A	2307	C	C6-N1-C2	-5.89	117.95	120.30
20	A	1878	U	N1-C2-O2	5.88	126.92	122.80
1	a	1183	C	N1-C2-O2	5.88	122.43	118.90
20	A	561	G	N3-C4-N9	5.88	129.53	126.00
1	a	769	C	C2-N1-C1'	5.88	125.26	118.80
20	A	1751	C	C6-N1-C2	-5.87	117.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	639	C	C6-N1-C1'	5.86	127.83	120.80
20	A	1996	U	N3-C2-O2	-5.86	118.10	122.20
1	a	346	G	C4-C5-N7	5.86	113.14	110.80
20	A	1479	C	C6-N1-C2	-5.85	117.96	120.30
20	A	1130	U	O4'-C1'-N1	5.85	112.88	108.20
20	A	2787	U	N3-C2-O2	-5.84	118.11	122.20
20	A	945	C	C2-N1-C1'	5.84	125.23	118.80
20	A	1349	U	C6-N1-C1'	-5.84	113.03	121.20
1	a	108	U	C2-N1-C1'	5.83	124.70	117.70
1	a	148	G	O4'-C1'-N9	5.83	112.87	108.20
20	A	495	C	N1-C2-O2	5.83	122.40	118.90
20	A	2007	U	N1-C2-O2	5.83	126.88	122.80
20	A	962	C	C6-N1-C2	-5.83	117.97	120.30
20	A	638	C	C2-N1-C1'	5.82	125.20	118.80
20	A	2240	C	N3-C2-O2	-5.82	117.83	121.90
20	A	848	G	C5-C6-O6	5.82	132.09	128.60
1	a	55	C	C2-N1-C1'	5.81	125.19	118.80
1	a	427	A	P-O3'-C3'	5.81	126.67	119.70
20	A	602	C	N3-C2-O2	-5.80	117.84	121.90
20	A	1758	C	N1-C2-O2	5.80	122.38	118.90
1	a	597	C	N3-C2-O2	-5.80	117.84	121.90
1	a	424	U	N3-C2-O2	-5.79	118.15	122.20
20	A	1045	C	N1-C2-O2	5.79	122.37	118.90
1	a	639	C	C6-N1-C2	-5.78	117.99	120.30
1	a	644	A	C4-N9-C1'	5.78	136.70	126.30
20	A	47	C	C2-N1-C1'	5.78	125.15	118.80
20	A	1955	C	N1-C2-O2	5.78	122.36	118.90
1	a	862	C	N1-C2-O2	5.77	122.36	118.90
21	B	101	U	N1-C2-O2	5.77	126.84	122.80
19	t	49	LEU	CA-CB-CG	5.77	128.57	115.30
20	A	956	C	N3-C2-O2	-5.77	117.86	121.90
20	A	1081	U	N1-C2-O2	5.76	126.84	122.80
20	A	1948	C	C6-N1-C2	-5.76	117.99	120.30
20	A	901	U	C6-N1-C1'	-5.75	113.14	121.20
20	A	162	A	C8-N9-C4	-5.75	103.50	105.80
1	a	860	C	N3-C2-O2	-5.75	117.87	121.90
20	A	2812	A	P-O3'-C3'	5.75	126.60	119.70
1	a	386	G	P-O3'-C3'	5.75	126.60	119.70
20	A	2142	C	N1-C2-O2	5.75	122.35	118.90
20	A	638	C	C6-N1-C2	-5.74	118.00	120.30
20	A	848	G	N1-C6-O6	-5.74	116.45	119.90
20	A	2518	U	C5-C6-N1	5.74	125.57	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	943	U	C2-N1-C1'	5.74	124.58	117.70
1	a	199	C	N3-C2-O2	-5.73	117.89	121.90
20	A	897	G	C8-N9-C1'	5.73	134.45	127.00
22	C	91	ILE	CG1-CB-CG2	-5.73	98.79	111.40
1	a	1548	U	C5-C6-N1	5.73	125.56	122.70
1	a	419	G	C4-N9-C1'	5.72	133.94	126.50
20	A	2142	C	C6-N1-C2	-5.72	118.01	120.30
20	A	679	C	C5-C6-N1	5.72	123.86	121.00
1	a	107	G	C5-C6-O6	5.72	132.03	128.60
20	A	1197	G	C6-C5-N7	-5.71	126.97	130.40
20	A	1969	U	C5-C6-N1	-5.71	119.85	122.70
1	a	720	U	N3-C2-O2	-5.71	118.21	122.20
1	a	578	A	C8-N9-C1'	-5.70	117.44	127.70
20	A	272	C	N1-C2-O2	5.70	122.32	118.90
1	a	927	U	N3-C2-O2	-5.69	118.22	122.20
20	A	1723	U	N3-C2-O2	-5.69	118.22	122.20
20	A	2208	C	C2-N1-C1'	5.69	125.06	118.80
20	A	1802	C	C6-N1-C2	-5.69	118.02	120.30
20	A	571	A	C2-N3-C4	5.69	113.44	110.60
20	A	1379	G	N3-C4-C5	-5.68	125.76	128.60
20	A	310	G	C8-N9-C1'	-5.68	119.61	127.00
20	A	849	G	C8-N9-C4	-5.68	104.13	106.40
20	A	1489	C	C2-N1-C1'	5.68	125.05	118.80
20	A	495	C	C2-N1-C1'	5.68	125.05	118.80
1	a	766	U	N3-C2-O2	-5.68	118.23	122.20
20	A	561	G	C6-C5-N7	-5.67	127.00	130.40
20	A	1128	A	C5-C6-N6	-5.67	119.16	123.70
20	A	549	C	C5-C6-N1	5.67	123.84	121.00
20	A	931	C	N1-C2-O2	5.66	122.30	118.90
20	A	1075	U	N1-C2-O2	5.66	126.76	122.80
1	a	384	C	C2-N1-C1'	5.65	125.02	118.80
1	a	952	C	C2-N1-C1'	5.65	125.02	118.80
1	a	1082	C	C6-N1-C1'	-5.65	114.02	120.80
1	a	660	G	C4-N9-C1'	5.65	133.84	126.50
20	A	780	C	C6-N1-C2	-5.64	118.04	120.30
20	A	1140	C	N1-C2-O2	5.64	122.29	118.90
1	a	267	U	N3-C2-O2	-5.64	118.25	122.20
1	a	204	G	N1-C6-O6	-5.64	116.52	119.90
1	a	968	U	N1-C2-O2	5.63	126.75	122.80
20	A	1699	C	C6-N1-C2	-5.63	118.05	120.30
20	A	1100	U	N3-C4-O4	5.63	123.34	119.40
20	A	413	U	N1-C2-O2	5.62	126.73	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	973	U	N1-C2-O2	5.62	126.73	122.80
20	A	1350	C	C5-C6-N1	5.62	123.81	121.00
20	A	1502	G	P-O3'-C3'	5.62	126.45	119.70
20	A	1723	U	C2-N1-C1'	5.62	124.44	117.70
1	a	862	C	C2-N1-C1'	5.61	124.97	118.80
20	A	2030	U	N3-C2-O2	-5.61	118.27	122.20
20	A	1902	G	O4'-C1'-N9	5.61	112.69	108.20
20	A	2724	C	N3-C2-O2	-5.61	117.97	121.90
21	B	96	G	C8-N9-C1'	-5.61	119.71	127.00
20	A	1936	G	N3-C4-N9	-5.60	122.64	126.00
20	A	823	A	C2-N3-C4	5.60	113.40	110.60
20	A	730	C	C2-N1-C1'	5.59	124.95	118.80
20	A	1505	C	N3-C2-O2	-5.59	117.98	121.90
20	A	1362	U	N3-C2-O2	-5.59	118.28	122.20
20	A	933	G	N3-C4-C5	-5.59	125.81	128.60
20	A	1399	C	C6-N1-C2	-5.59	118.06	120.30
3	d	26	LEU	CA-CB-CG	5.59	128.15	115.30
20	A	654	A	N7-C8-N9	-5.59	111.01	113.80
20	A	1502	G	OP1-P-O3'	5.59	117.49	105.20
20	A	310	G	N3-C4-C5	-5.58	125.81	128.60
1	a	156	U	C2-N1-C1'	5.58	124.40	117.70
1	a	279	C	N3-C2-O2	-5.58	117.99	121.90
1	a	424	U	N1-C2-O2	5.58	126.71	122.80
21	B	101	U	N3-C2-O2	-5.58	118.29	122.20
1	a	67	U	N3-C2-O2	-5.58	118.30	122.20
20	A	573	U	C5-C6-N1	5.57	125.49	122.70
20	A	1350	C	N1-C2-O2	5.56	122.24	118.90
20	A	1479	C	C2-N1-C1'	5.56	124.92	118.80
1	a	529	C	C2-N1-C1'	5.56	124.92	118.80
1	a	1091	U	N1-C2-O2	5.56	126.69	122.80
20	A	475	C	N1-C2-O2	5.56	122.23	118.90
20	A	1434	C	C5-C6-N1	5.56	123.78	121.00
1	a	109	G	N1-C6-O6	-5.55	116.57	119.90
20	A	2836	G	C6-C5-N7	-5.55	127.07	130.40
1	a	720	U	N1-C2-O2	5.55	126.68	122.80
1	a	585	G	C4-N9-C1'	5.54	133.71	126.50
1	a	1094	U	N1-C2-O2	5.54	126.68	122.80
20	A	2317	G	P-O3'-C3'	5.54	126.35	119.70
1	a	660	G	N3-C4-C5	-5.54	125.83	128.60
20	A	571	A	C4-N9-C1'	5.54	136.27	126.30
1	a	952	C	C6-N1-C2	-5.54	118.09	120.30
1	a	6	G	O4'-C1'-N9	5.53	112.63	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	709	G	N3-C4-N9	5.53	129.32	126.00
20	A	2700	G	N3-C4-C5	-5.53	125.83	128.60
20	A	657	C	C6-N1-C2	-5.53	118.09	120.30
20	A	2050	C	N1-C2-O2	5.53	122.22	118.90
1	a	56	A	N3-C4-N9	5.53	131.82	127.40
20	A	2825	C	C2-N1-C1'	5.53	124.88	118.80
1	a	279	C	N1-C2-O2	5.52	122.21	118.90
1	a	968	U	C2-N1-C1'	5.52	124.32	117.70
20	A	2670	U	N3-C2-O2	-5.52	118.34	122.20
1	a	560	C	C5-C6-N1	5.52	123.76	121.00
20	A	1948	C	N3-C2-O2	-5.52	118.04	121.90
1	a	148	G	C4-N9-C1'	5.51	133.67	126.50
1	a	1043	C	C5-C6-N1	5.51	123.76	121.00
20	A	1175	C	N1-C2-O2	5.51	122.21	118.90
20	A	137	U	N3-C2-O2	-5.51	118.34	122.20
20	A	2596	G	N3-C4-C5	-5.51	125.84	128.60
1	a	543	C	C6-N1-C2	-5.51	118.10	120.30
1	a	1040	U	C2-N1-C1'	5.51	124.31	117.70
1	a	627	C	C2-N1-C1'	5.51	124.86	118.80
1	a	660	G	N3-C4-N9	5.50	129.30	126.00
20	A	423	C	N3-C2-O2	-5.50	118.05	121.90
20	A	925	C	C5-C6-N1	5.50	123.75	121.00
20	A	1045	C	C2-N1-C1'	5.50	124.85	118.80
20	A	1831	G	C4-N9-C1'	5.50	133.65	126.50
1	a	875	C	C2-N1-C1'	5.50	124.85	118.80
20	A	209	U	N1-C2-O2	5.49	126.65	122.80
1	a	143	C	N1-C2-O2	5.49	122.19	118.90
20	A	1561	U	N1-C2-O2	5.49	126.64	122.80
1	a	392	G	N3-C4-C5	-5.49	125.86	128.60
1	a	1053	C	C2-N1-C1'	5.49	124.84	118.80
20	A	1561	U	N3-C2-O2	-5.48	118.36	122.20
20	A	1092	C	N3-C2-O2	-5.48	118.06	121.90
20	A	121	G	C6-C5-N7	-5.48	127.11	130.40
1	a	754	C	C5-C6-N1	5.47	123.74	121.00
20	A	2090	U	N3-C2-O2	-5.47	118.37	122.20
1	a	421	G	N3-C4-N9	5.47	129.28	126.00
20	A	1408	U	N3-C2-O2	-5.47	118.37	122.20
20	A	2408	C	N1-C2-O2	5.47	122.18	118.90
20	A	586	A	N1-C6-N6	-5.46	115.32	118.60
20	A	2206	C	N1-C2-O2	5.46	122.18	118.90
1	a	826	C	C5-C6-N1	5.46	123.73	121.00
11	l	131	GLY	N-CA-C	5.46	126.75	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	145	U	N3-C2-O2	-5.45	118.38	122.20
20	A	823	A	C4-N9-C1'	5.45	136.10	126.30
20	A	1157	C	N1-C2-O2	5.45	122.17	118.90
20	A	164	U	C2-N3-C4	-5.44	123.73	127.00
20	A	1047	C	C2-N1-C1'	5.44	124.79	118.80
1	a	734	C	N1-C2-O2	5.44	122.16	118.90
20	A	1492	G	N3-C4-N9	-5.44	122.74	126.00
20	A	1603	C	OP2-P-O3'	5.44	117.16	105.20
20	A	657	C	C2-N1-C1'	5.43	124.78	118.80
20	A	1689	A	N3-C4-N9	5.43	131.75	127.40
20	A	1216	G	N3-C4-N9	5.42	129.25	126.00
1	a	199	C	N1-C2-O2	5.42	122.15	118.90
20	A	943	U	N1-C2-O2	5.41	126.59	122.80
20	A	1435	C	C2-N1-C1'	5.41	124.76	118.80
1	a	995	C	C6-N1-C2	-5.41	118.14	120.30
1	a	952	C	C5-C6-N1	5.41	123.70	121.00
1	a	997	U	C6-N1-C1'	-5.41	113.62	121.20
20	A	2786	C	C5-C6-N1	5.41	123.70	121.00
1	a	250	C	N3-C2-O2	-5.41	118.12	121.90
1	a	140	A	C4-N9-C1'	5.40	136.03	126.30
1	a	107	G	N1-C6-O6	-5.40	116.66	119.90
20	A	137	U	N1-C2-O2	5.40	126.58	122.80
1	a	55	C	C5-C6-N1	5.40	123.70	121.00
1	a	632	G	C5-C6-O6	5.40	131.84	128.60
20	A	1928	C	C2-N1-C1'	5.39	124.73	118.80
20	A	2121	C	N3-C2-O2	-5.39	118.12	121.90
20	A	2697	C	C6-N1-C2	-5.39	118.14	120.30
20	A	2753	U	C2-N1-C1'	5.39	124.16	117.70
1	a	1040	U	N3-C2-O2	-5.38	118.43	122.20
20	A	1092	C	C6-N1-C2	-5.38	118.15	120.30
1	a	322	U	C6-N1-C2	-5.38	117.77	121.00
20	A	716	A	O4'-C1'-N9	5.38	112.51	108.20
1	a	419	G	N3-C4-C5	-5.38	125.91	128.60
20	A	2552	C	C6-N1-C2	-5.38	118.15	120.30
1	a	1005	U	N3-C2-O2	-5.38	118.43	122.20
20	A	2488	C	N3-C2-O2	-5.38	118.14	121.90
19	t	81	LEU	CA-CB-CG	5.37	127.66	115.30
20	A	169	A	O4'-C1'-N9	5.37	112.50	108.20
20	A	730	C	C5-C6-N1	5.37	123.69	121.00
1	a	1183	C	C6-N1-C1'	-5.37	114.36	120.80
21	B	24	U	N3-C2-O2	-5.37	118.44	122.20
20	A	2020	C	C2-N1-C1'	5.37	124.70	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1024	G	C8-N9-C1'	-5.36	120.03	127.00
20	A	209	U	C2-N1-C1'	5.36	124.13	117.70
1	a	190	A	C8-N9-C4	-5.35	103.66	105.80
1	a	199	C	C6-N1-C2	-5.35	118.16	120.30
20	A	2020	C	C6-N1-C2	-5.35	118.16	120.30
1	a	927	U	N1-C2-O2	5.35	126.54	122.80
20	A	476	C	C6-N1-C2	-5.35	118.16	120.30
20	A	509	G	N7-C8-N9	5.35	115.77	113.10
1	a	146	C	C5-C6-N1	5.34	123.67	121.00
1	a	516	C	N3-C4-N4	-5.34	114.26	118.00
20	A	1362	U	N1-C2-O2	5.34	126.54	122.80
31	O	41	ARG	CB-CG-CD	-5.33	97.73	111.60
1	a	1446	C	N1-C2-O2	5.33	122.10	118.90
20	A	1689	A	C4-N9-C1'	5.33	135.90	126.30
20	A	906	C	C6-N1-C1'	-5.33	114.40	120.80
20	A	2262	C	C2-N1-C1'	5.33	124.66	118.80
20	A	2592	G	N1-C6-O6	-5.33	116.70	119.90
1	a	644	A	N7-C8-N9	5.32	116.46	113.80
20	A	121	G	N3-C4-N9	5.32	129.19	126.00
20	A	956	C	C6-N1-C2	-5.32	118.17	120.30
20	A	955	C	C6-N1-C2	-5.31	118.17	120.30
20	A	2206	C	N3-C2-O2	-5.31	118.18	121.90
1	a	1148	C	N1-C2-O2	5.31	122.08	118.90
20	A	1408	U	N1-C2-O2	5.31	126.52	122.80
20	A	1948	C	C6-N1-C1'	-5.31	114.43	120.80
20	A	1128	A	N1-C6-N6	5.31	121.78	118.60
20	A	1638	C	C2-N1-C1'	5.31	124.64	118.80
20	A	569	C	N1-C2-O2	5.30	122.08	118.90
20	A	1379	G	C8-N9-C1'	-5.30	120.11	127.00
20	A	939	C	N3-C2-O2	-5.30	118.19	121.90
20	A	2595	G	C4-N9-C1'	5.30	133.39	126.50
1	a	66	C	C5-C6-N1	5.30	123.65	121.00
1	a	234	C	N1-C2-O2	5.30	122.08	118.90
1	a	860	C	C6-N1-C2	-5.29	118.18	120.30
21	B	32	U	P-O3'-C3'	5.29	126.05	119.70
20	A	897	G	C6-C5-N7	5.29	133.57	130.40
20	A	1317	G	N3-C4-N9	5.29	129.17	126.00
20	A	1719	A	C8-N9-C4	-5.29	103.69	105.80
1	a	66	C	C2-N1-C1'	5.29	124.62	118.80
20	A	67	C	N1-C2-O2	5.29	122.07	118.90
20	A	1295	C	N3-C2-O2	-5.29	118.20	121.90
20	A	1304	U	C5-C6-N1	5.29	125.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	423	C	C6-N1-C2	-5.28	118.19	120.30
20	A	1569	G	N3-C4-N9	-5.28	122.83	126.00
20	A	1369	C	C6-N1-C2	-5.28	118.19	120.30
1	a	51	C	N1-C2-O2	5.28	122.06	118.90
20	A	1574	C	C2-N1-C1'	5.28	124.60	118.80
20	A	2794	G	N3-C4-N9	5.28	129.17	126.00
20	A	1906	C	C6-N1-C2	-5.27	118.19	120.30
20	A	2858	U	C2-N1-C1'	5.27	124.02	117.70
20	A	237	U	N3-C2-O2	-5.26	118.52	122.20
20	A	2188	C	N3-C2-O2	-5.26	118.22	121.90
20	A	835	C	C5-C6-N1	5.26	123.63	121.00
1	a	331	C	C2-N1-C1'	5.25	124.58	118.80
20	A	1853	G	C4-N9-C1'	5.25	133.33	126.50
20	A	2836	G	C4-C5-N7	5.25	112.90	110.80
21	B	35	C	N1-C2-O2	5.25	122.05	118.90
1	a	634	U	N3-C2-O2	-5.25	118.52	122.20
20	A	2854	G	N3-C4-N9	5.25	129.15	126.00
20	A	2090	U	C2-N1-C1'	5.25	124.00	117.70
20	A	1768	C	C6-N1-C2	-5.25	118.20	120.30
20	A	549	C	C6-N1-C2	-5.24	118.20	120.30
20	A	602	C	C2-N1-C1'	5.24	124.57	118.80
20	A	992	G	N3-C4-N9	5.24	129.15	126.00
20	A	121	G	C4-C5-N7	5.24	112.90	110.80
20	A	960	U	N1-C2-O2	5.24	126.47	122.80
20	A	1981	C	C2-N1-C1'	5.24	124.56	118.80
20	A	77	C	C6-N1-C2	-5.24	118.20	120.30
20	A	823	A	C8-N9-C4	-5.24	103.70	105.80
20	A	325	U	N3-C2-O2	-5.24	118.53	122.20
20	A	2606	G	N3-C4-N9	5.24	129.14	126.00
20	A	2021	U	N3-C2-O2	-5.23	118.54	122.20
20	A	561	G	C4-N9-C1'	5.23	133.29	126.50
1	a	498	C	C2-N1-C1'	5.22	124.55	118.80
20	A	709	G	C8-N9-C1'	-5.22	120.21	127.00
1	a	148	G	C8-N9-C4	-5.22	104.31	106.40
20	A	1492	G	N3-C4-C5	5.22	131.21	128.60
20	A	943	U	N3-C2-O2	-5.22	118.55	122.20
20	A	2474	U	N1-C2-O2	5.22	126.45	122.80
1	a	141	C	C2-N1-C1'	5.21	124.54	118.80
1	a	148	G	N3-C4-N9	5.21	129.13	126.00
1	a	418	C	C6-N1-C1'	-5.21	114.55	120.80
1	a	71	U	N1-C2-O2	5.20	126.44	122.80
20	A	4	U	C2-N1-C1'	5.20	123.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	2808	C	C6-N1-C2	-5.20	118.22	120.30
1	a	644	A	C8-N9-C1'	-5.20	118.34	127.70
20	A	607	G	N3-C4-N9	5.20	129.12	126.00
20	A	1108	G	N3-C4-C5	-5.20	126.00	128.60
20	A	499	U	N3-C2-O2	-5.20	118.56	122.20
20	A	2570	C	C2-N1-C1'	5.20	124.52	118.80
20	A	1723	U	N1-C2-O2	5.19	126.44	122.80
20	A	2552	C	C5-C6-N1	5.19	123.60	121.00
20	A	2766	C	C6-N1-C2	-5.19	118.22	120.30
20	A	549	C	N3-C2-O2	-5.18	118.27	121.90
1	a	639	C	N3-C2-O2	-5.18	118.27	121.90
20	A	1689	A	N3-C4-C5	-5.18	123.17	126.80
20	A	1197	G	C4-C5-N7	5.18	112.87	110.80
1	a	1022	C	N3-C2-O2	-5.18	118.28	121.90
20	A	2278	C	N3-C2-O2	-5.18	118.28	121.90
1	a	392	G	N3-C4-N9	5.18	129.11	126.00
1	a	634	U	N1-C2-O2	5.18	126.42	122.80
20	A	1603	C	P-O3'-C3'	5.17	125.91	119.70
1	a	71	U	N3-C2-O2	-5.17	118.58	122.20
1	a	559	G	P-O3'-C3'	5.17	125.90	119.70
20	A	77	C	C5-C6-N1	5.17	123.58	121.00
20	A	167	A	N1-C2-N3	-5.16	126.72	129.30
20	A	211	C	N1-C2-O2	5.16	122.00	118.90
20	A	550	U	C2-N1-C1'	5.16	123.90	117.70
20	A	1034	C	C6-N1-C2	-5.16	118.23	120.30
20	A	1501	A	C2-N3-C4	5.16	113.18	110.60
1	a	754	C	C6-N1-C2	-5.16	118.24	120.30
1	a	1022	C	C2-N1-C1'	5.16	124.47	118.80
20	A	1317	G	C4-N9-C1'	5.16	133.21	126.50
20	A	2670	U	N1-C2-O2	5.16	126.41	122.80
20	A	621	C	C6-N1-C2	-5.16	118.24	120.30
21	B	28	C	N1-C2-O2	5.16	121.99	118.90
1	a	392	G	C4-N9-C1'	5.15	133.20	126.50
1	a	346	G	C6-C5-N7	-5.15	127.31	130.40
1	a	559	G	N7-C8-N9	5.15	115.67	113.10
20	A	2188	C	N1-C2-O2	5.15	121.99	118.90
21	B	35	C	N3-C2-O2	-5.15	118.30	121.90
20	A	588	G	N3-C4-C5	-5.15	126.03	128.60
21	B	73	U	N3-C2-O2	-5.14	118.60	122.20
20	A	709	G	N3-C4-C5	-5.14	126.03	128.60
20	A	1642	C	C2-N1-C1'	5.14	124.46	118.80
20	A	2057	C	C2-N1-C1'	5.14	124.46	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	790	G	N3-C2-N2	-5.14	116.30	119.90
20	A	509	G	C5-N7-C8	-5.14	101.73	104.30
20	A	1399	C	C5-C6-N1	5.13	123.57	121.00
20	A	638	C	C5-C6-N1	5.13	123.57	121.00
20	A	742	U	N3-C2-O2	-5.13	118.61	122.20
20	A	1106	U	C2-N1-C1'	5.13	123.86	117.70
20	A	1278	C	C2-N1-C1'	5.13	124.44	118.80
20	A	1703	C	C5-C6-N1	5.13	123.57	121.00
20	A	2819	U	C2-N1-C1'	5.13	123.86	117.70
20	A	939	C	N1-C2-O2	5.13	121.98	118.90
1	a	585	G	N3-C4-N9	5.13	129.08	126.00
20	A	2812	A	OP1-P-O3'	5.13	116.48	105.20
20	A	1149	C	N1-C2-O2	5.13	121.98	118.90
20	A	286	U	C5-C6-N1	5.12	125.26	122.70
20	A	769	G	N3-C4-N9	-5.12	122.93	126.00
34	R	13	ARG	CB-CG-CD	-5.12	98.28	111.60
1	a	673	G	C8-N9-C4	-5.12	104.35	106.40
1	a	790	G	C2-N3-C4	-5.12	109.34	111.90
20	A	2896	C	C6-N1-C2	-5.12	118.25	120.30
1	a	1162	C	N1-C2-O2	5.11	121.97	118.90
20	A	1550	U	N1-C2-O2	5.11	126.38	122.80
20	A	655	G	N9-C4-C5	-5.11	103.36	105.40
20	A	1029	G	C4-N9-C1'	5.11	133.14	126.50
1	a	790	G	N3-C4-C5	5.11	131.15	128.60
20	A	2734	U	C2-N1-C1'	5.11	123.83	117.70
20	A	201	C	N1-C2-O2	5.11	121.96	118.90
20	A	1149	C	C2-N1-C1'	5.11	124.42	118.80
1	a	704	C	C5-C6-N1	5.10	123.55	121.00
1	a	108	U	C5-C4-O4	-5.10	122.84	125.90
20	A	975	U	N1-C2-O2	5.10	126.37	122.80
1	a	1442	C	C6-N1-C2	-5.10	118.26	120.30
20	A	1350	C	C6-N1-C1'	-5.10	114.68	120.80
20	A	1216	G	N3-C4-C5	-5.09	126.05	128.60
1	a	267	U	N1-C2-O2	5.09	126.36	122.80
1	a	1318	C	N1-C2-O2	5.09	121.95	118.90
20	A	963	C	C6-N1-C1'	5.09	126.90	120.80
20	A	1350	C	N3-C2-O2	-5.09	118.34	121.90
20	A	2062	G	C4-N9-C1'	5.08	133.11	126.50
1	a	867	C	N3-C2-O2	-5.08	118.35	121.90
20	A	2474	U	N3-C2-O2	-5.08	118.65	122.20
1	a	105	G	P-O3'-C3'	5.08	125.79	119.70
3	d	17	ILE	CG1-CB-CG2	-5.08	100.23	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	325	U	C2-N1-C1'	5.08	123.79	117.70
20	A	1928	C	C6-N1-C2	-5.07	118.27	120.30
20	A	2077	C	N1-C2-O2	5.07	121.94	118.90
20	A	848	G	N3-C4-N9	-5.07	122.96	126.00
20	A	769	G	C2-N3-C4	-5.07	109.37	111.90
20	A	1434	C	C6-N1-C2	-5.06	118.28	120.30
1	a	409	G	C4-N9-C1'	5.06	133.08	126.50
20	A	2138	G	C4-N9-C1'	5.06	133.08	126.50
1	a	415	C	N3-C2-O2	-5.06	118.36	121.90
1	a	1183	C	O4'-C1'-N1	5.06	112.25	108.20
20	A	261	C	C2-N1-C1'	5.06	124.36	118.80
20	A	992	G	C4-N9-C1'	5.06	133.07	126.50
20	A	1234	C	C6-N1-C2	-5.06	118.28	120.30
1	a	178	A	C8-N9-C4	-5.05	103.78	105.80
1	a	1005	U	N1-C2-O2	5.05	126.34	122.80
1	a	1465	U	C2-N1-C1'	5.05	123.77	117.70
1	a	790	G	C8-N9-C1'	5.05	133.56	127.00
20	A	1047	C	C5-C6-N1	5.04	123.52	121.00
20	A	2576	U	N3-C2-O2	-5.04	118.67	122.20
1	a	649	C	C5-C6-N1	5.04	123.52	121.00
20	A	2897	G	C4-N9-C1'	5.04	133.05	126.50
1	a	1306	C	N1-C2-O2	5.04	121.92	118.90
20	A	1128	A	N3-C4-N9	5.04	131.43	127.40
20	A	2785	C	C2-N1-C1'	5.04	124.34	118.80
20	A	1511	C	N3-C2-O2	-5.03	118.38	121.90
1	a	109	G	N3-C2-N2	-5.03	116.38	119.90
1	a	1173	C	C6-N1-C1'	-5.03	114.77	120.80
1	a	639	C	N1-C2-N3	5.02	122.72	119.20
20	A	2311	C	N3-C2-O2	-5.02	118.39	121.90
21	B	24	U	N1-C2-O2	5.02	126.31	122.80
20	A	1584	G	OP2-P-O3'	5.02	116.24	105.20
1	a	504	C	N1-C2-O2	5.02	121.91	118.90
20	A	1634	A	N3-C4-N9	5.02	131.41	127.40
20	A	2836	G	C5-N7-C8	-5.02	101.79	104.30
1	a	1077	G	C4-N9-C1'	5.02	133.02	126.50
1	a	464	A	C8-N9-C4	-5.01	103.80	105.80
20	A	638	C	N1-C2-O2	5.01	121.91	118.90
20	A	121	G	C4-N9-C1'	5.01	133.02	126.50
20	A	1132	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1125	C	N3-C2-O2	-5.01	118.39	121.90
1	a	712	U	N3-C2-O2	-5.01	118.69	122.20
20	A	1115	C	N1-C2-O2	5.01	121.90	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	636	A	C2-N3-C4	5.00	113.10	110.60
20	A	2826	C	C6-N1-C2	-5.00	118.30	120.30
1	a	190	A	C5-N7-C8	-5.00	101.40	103.90
1	a	632	G	C8-N9-C1'	5.00	133.50	127.00
1	a	1038	C	N3-C2-O2	-5.00	118.40	121.90
20	A	778	C	C2-N1-C1'	5.00	124.30	118.80
1	a	530	G	C8-N9-C1'	-5.00	120.50	127.00
20	A	890	A	P-O3'-C3'	5.00	125.70	119.70
20	A	1234	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	4	3	ARG	Peptide
22	C	154	LEU	Peptide
22	C	195	VAL	Peptide
23	D	53	TYR	Peptide
23	D	89	GLY	Peptide
24	E	45	ARG	Peptide
24	E	80	SER	Peptide
25	F	121	ALA	Peptide
26	G	47	GLY	Peptide
26	G	61	MET	Peptide
27	K	131	HIS	Peptide
27	K	45	PHE	Peptide
29	M	30	THR	Peptide
29	M	85	PHE	Peptide
29	M	97	LYS	Peptide
30	N	133	LYS	Peptide
30	N	8	LYS	Peptide
31	O	22	THR	Peptide
31	O	77	ASP	Peptide
32	P	22	ILE	Peptide
32	P	30	ARG	Peptide
32	P	93	PHE	Peptide
35	S	100	ILE	Peptide
35	S	50	ALA	Peptide
37	U	50	VAL	Peptide
37	U	62	PHE	Peptide
38	V	72	ASP	Peptide
38	V	87	ASP	Peptide

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Mol	Chain	Res	Type	Group
39	W	15	ARG	Peptide
40	X	49	GLN	Peptide
41	Y	21	ALA	Peptide
11	l	130	TYR	Peptide
11	l	37	ASN	Peptide
12	m	43	VAL	Peptide
16	q	73	THR	Peptide
19	t	66	ILE	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c	202/204 (99%)	178 (88%)	24 (12%)	0	100	100
3	d	199/201 (99%)	169 (85%)	30 (15%)	0	100	100
4	e	161/163 (99%)	142 (88%)	19 (12%)	0	100	100
5	f	95/97 (98%)	88 (93%)	7 (7%)	0	100	100
6	g	152/154 (99%)	138 (91%)	14 (9%)	0	100	100
7	h	129/131 (98%)	116 (90%)	13 (10%)	0	100	100
8	i	126/128 (98%)	110 (87%)	15 (12%)	1 (1%)	19	58
9	j	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
10	k	115/117 (98%)	98 (85%)	17 (15%)	0	100	100
11	l	134/136 (98%)	106 (79%)	27 (20%)	1 (1%)	22	61
12	m	110/112 (98%)	86 (78%)	24 (22%)	0	100	100
13	n	58/60 (97%)	53 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	o	86/88 (98%)	79 (92%)	7 (8%)	0	100	100
15	p	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
16	q	81/83 (98%)	67 (83%)	14 (17%)	0	100	100
17	r	64/66 (97%)	53 (83%)	11 (17%)	0	100	100
18	s	76/78 (97%)	60 (79%)	16 (21%)	0	100	100
19	t	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
22	C	273/275 (99%)	236 (86%)	37 (14%)	0	100	100
23	D	205/207 (99%)	182 (89%)	22 (11%)	1 (0%)	29	68
24	E	204/206 (99%)	175 (86%)	29 (14%)	0	100	100
25	F	175/177 (99%)	149 (85%)	26 (15%)	0	100	100
26	G	172/176 (98%)	145 (84%)	25 (14%)	2 (1%)	13	50
27	K	142/145 (98%)	124 (87%)	18 (13%)	0	100	100
28	L	120/122 (98%)	98 (82%)	22 (18%)	0	100	100
29	M	143/146 (98%)	105 (73%)	35 (24%)	3 (2%)	7	38
30	N	137/141 (97%)	111 (81%)	26 (19%)	0	100	100
31	O	119/123 (97%)	95 (80%)	24 (20%)	0	100	100
32	P	115/117 (98%)	100 (87%)	15 (13%)	0	100	100
33	Q	110/114 (96%)	98 (89%)	12 (11%)	0	100	100
34	R	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
35	S	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
36	T	110/112 (98%)	95 (86%)	15 (14%)	0	100	100
37	U	87/89 (98%)	72 (83%)	13 (15%)	2 (2%)	6	36
38	V	99/101 (98%)	75 (76%)	21 (21%)	3 (3%)	4	30
39	W	92/94 (98%)	74 (80%)	17 (18%)	1 (1%)	14	52
40	X	73/76 (96%)	64 (88%)	9 (12%)	0	100	100
41	Y	52/54 (96%)	44 (85%)	8 (15%)	0	100	100
42	Z	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
43	0	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
44	1	81/83 (98%)	60 (74%)	21 (26%)	0	100	100
45	2	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
46	3	47/49 (96%)	45 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	4	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
48	5	62/64 (97%)	55 (89%)	7 (11%)	0	100	100
49	6	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
All	All	5128/5235 (98%)	4406 (86%)	708 (14%)	14 (0%)	44	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	G	48	ASN
29	M	95	VAL
29	M	98	GLU
39	W	16	SER
11	l	131	GLY
26	G	47	GLY
38	V	73	PRO
38	V	88	GLY
37	U	51	ALA
23	D	90	GLU
38	V	72	ASP
8	i	41	HIS
37	U	52	ASN
29	M	94	VAL

### 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	
2	c	162/162 (100%)	162 (100%)	0	100	100
3	d	175/175 (100%)	173 (99%)	2 (1%)	73	88
4	e	126/126 (100%)	126 (100%)	0	100	100
5	f	86/86 (100%)	86 (100%)	0	100	100
6	g	131/131 (100%)	131 (100%)	0	100	100
7	h	112/112 (100%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	101/101 (100%)	100 (99%)	1 (1%)	76	88
9	j	90/90 (100%)	88 (98%)	2 (2%)	52	78
10	k	91/91 (100%)	90 (99%)	1 (1%)	73	88
11	l	118/118 (100%)	115 (98%)	3 (2%)	47	75
12	m	95/95 (100%)	95 (100%)	0	100	100
13	n	51/51 (100%)	50 (98%)	1 (2%)	55	79
14	o	78/78 (100%)	76 (97%)	2 (3%)	46	74
15	p	79/79 (100%)	77 (98%)	2 (2%)	47	75
16	q	76/76 (100%)	74 (97%)	2 (3%)	46	74
17	r	57/57 (100%)	54 (95%)	3 (5%)	22	55
18	s	68/68 (100%)	67 (98%)	1 (2%)	65	84
19	t	62/62 (100%)	62 (100%)	0	100	100
22	C	224/225 (100%)	223 (100%)	1 (0%)	91	96
23	D	168/170 (99%)	164 (98%)	4 (2%)	49	76
24	E	172/172 (100%)	170 (99%)	2 (1%)	71	87
25	F	154/154 (100%)	154 (100%)	0	100	100
26	G	145/146 (99%)	145 (100%)	0	100	100
27	K	121/122 (99%)	120 (99%)	1 (1%)	81	91
28	L	98/98 (100%)	98 (100%)	0	100	100
29	M	111/112 (99%)	111 (100%)	0	100	100
30	N	112/112 (100%)	110 (98%)	2 (2%)	59	81
31	O	105/105 (100%)	104 (99%)	1 (1%)	76	88
32	P	91/91 (100%)	91 (100%)	0	100	100
33	Q	94/97 (97%)	94 (100%)	0	100	100
34	R	92/94 (98%)	92 (100%)	0	100	100
35	S	82/83 (99%)	82 (100%)	0	100	100
36	T	95/95 (100%)	95 (100%)	0	100	100
37	U	80/80 (100%)	78 (98%)	2 (2%)	47	75
38	V	85/85 (100%)	85 (100%)	0	100	100
39	W	85/85 (100%)	85 (100%)	0	100	100
40	X	60/61 (98%)	59 (98%)	1 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Y	47/47 (100%)	45 (96%)	2 (4%)	29	62
42	Z	55/55 (100%)	54 (98%)	1 (2%)	59	81
43	0	48/49 (98%)	48 (100%)	0	100	100
44	1	75/75 (100%)	74 (99%)	1 (1%)	69	86
45	2	46/46 (100%)	46 (100%)	0	100	100
46	3	49/49 (100%)	49 (100%)	0	100	100
47	4	39/39 (100%)	39 (100%)	0	100	100
48	5	51/51 (100%)	51 (100%)	0	100	100
49	6	35/35 (100%)	35 (100%)	0	100	100
All	All	4377/4391 (100%)	4339 (99%)	38 (1%)	79	90

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	d	14	ARG
3	d	58	ARG
8	i	14	ASN
9	j	5	LYS
9	j	16	ARG
10	k	93	ARG
11	l	32	LYS
11	l	127	ARG
11	l	134	ARG
13	n	26	ARG
14	o	54	ARG
14	o	89	ARG
15	p	9	ARG
15	p	90	LYS
16	q	5	ARG
16	q	6	ASN
17	r	13	LYS
17	r	57	ARG
17	r	65	ARG
18	s	6	LYS
22	C	257	TYR
23	D	57	ARG
23	D	119	PHE
23	D	159	ARG
23	D	168	ARG

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Mol	Chain	Res	Type
24	E	74	ARG
24	E	169	ASN
27	K	45	PHE
30	N	10	ARG
30	N	119	ARG
31	O	114	ARG
37	U	48	VAL
37	U	62	PHE
40	X	80	ARG
41	Y	17	ASN
41	Y	32	ASN
42	Z	26	PHE
44	1	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
3	d	86	ASN
6	g	68	ASN
6	g	106	ASN
6	g	114	HIS
8	i	14	ASN
8	i	75	GLN
9	j	56	HIS
9	j	97	ASN
12	m	76	ASN
13	n	10	ASN
16	q	6	ASN
16	q	50	HIS
18	s	22	GLN
22	C	53	HIS
22	C	95	HIS
22	C	128	ASN
22	C	153	GLN
22	C	232	HIS
23	D	14	GLN
23	D	37	GLN
24	E	29	ASN
24	E	49	HIS
24	E	75	GLN
24	E	169	ASN
25	F	27	GLN

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Mol	Chain	Res	Type
25	F	37	ASN
26	G	106	ASN
28	L	13	ASN
32	P	20	ASN
32	P	32	ASN
34	R	81	HIS
35	S	88	HIS
36	T	102	ASN
38	V	44	HIS
40	X	87	GLN
41	Y	17	ASN
41	Y	23	ASN
41	Y	32	ASN
44	1	75	ASN
45	2	32	ASN
45	2	40	HIS
47	4	8	ASN
48	5	4	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1528 (99%)	441 (28%)	0
20	A	2895/2903 (99%)	650 (22%)	20 (0%)
21	B	113/116 (97%)	26 (23%)	2 (1%)
All	All	4534/4547 (99%)	1117 (24%)	22 (0%)

All (1117) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	5	A
1	a	6	G
1	a	7	A
1	a	11	U
1	a	13	A
1	a	19	G
1	a	25	G
1	a	29	A
1	a	32	G
1	a	36	G
1	a	38	G

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Mol	Chain	Res	Type
1	a	41	G
1	a	44	C
1	a	45	C
1	a	46	U
1	a	47	A
1	a	48	A
1	a	51	C
1	a	61	G
1	a	62	A
1	a	63	A
1	a	64	C
1	a	67	U
1	a	68	U
1	a	69	C
1	a	72	U
1	a	73	C
1	a	74	C
1	a	75	U
1	a	97	G
1	a	104	G
1	a	105	G
1	a	106	A
1	a	107	G
1	a	109	G
1	a	112	G
1	a	113	G
1	a	114	A
1	a	125	A
1	a	126	C
1	a	135	A
1	a	136	A
1	a	139	U
1	a	140	A
1	a	142	C
1	a	143	C
1	a	148	G
1	a	149	A
1	a	150	G
1	a	156	U
1	a	159	C
1	a	163	U
1	a	165	G

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Mol	Chain	Res	Type
1	a	167	A
1	a	168	A
1	a	169	C
1	a	172	G
1	a	180	A
1	a	183	G
1	a	184	C
1	a	185	A
1	a	187	A
1	a	188	A
1	a	189	C
1	a	190	A
1	a	197	G
1	a	199	C
1	a	200	G
1	a	201	C
1	a	202	A
1	a	206	C
1	a	207	A
1	a	208	U
1	a	211	G
1	a	212	A
1	a	213	G
1	a	214	U
1	a	217	A
1	a	218	A
1	a	219	G
1	a	221	C
1	a	225	U
1	a	227	C
1	a	230	G
1	a	233	U
1	a	234	C
1	a	235	G
1	a	238	G
1	a	240	U
1	a	250	C
1	a	255	U
1	a	256	G
1	a	262	G
1	a	266	G
1	a	278	A

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Mol	Chain	Res	Type
1	a	281	G
1	a	282	C
1	a	289	A
1	a	295	C
1	a	304	G
1	a	308	A
1	a	313	A
1	a	323	C
1	a	330	A
1	a	336	A
1	a	343	C
1	a	345	C
1	a	347	G
1	a	360	C
1	a	362	G
1	a	367	C
1	a	368	A
1	a	369	G
1	a	374	A
1	a	378	A
1	a	381	C
1	a	382	U
1	a	384	C
1	a	387	C
1	a	388	A
1	a	390	U
1	a	392	G
1	a	393	A
1	a	396	A
1	a	397	A
1	a	398	A
1	a	399	G
1	a	403	G
1	a	405	C
1	a	412	A
1	a	413	C
1	a	416	C
1	a	417	G
1	a	418	C
1	a	419	G
1	a	421	G
1	a	424	U

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Mol	Chain	Res	Type
1	a	425	G
1	a	426	A
1	a	427	A
1	a	428	G
1	a	429	A
1	a	430	A
1	a	435	U
1	a	437	C
1	a	438	G
1	a	439	G
1	a	443	G
1	a	444	U
1	a	446	A
1	a	448	A
1	a	450	U
1	a	451	C
1	a	453	G
1	a	454	U
1	a	456	G
1	a	457	U
1	a	459	A
1	a	462	G
1	a	463	A
1	a	465	G
1	a	467	A
1	a	468	C
1	a	469	A
1	a	470	A
1	a	471	G
1	a	475	G
1	a	476	U
1	a	477	U
1	a	478	A
1	a	479	G
1	a	480	U
1	a	481	A
1	a	483	C
1	a	485	G
1	a	486	A
1	a	487	A
1	a	488	C
1	a	489	G

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Mol	Chain	Res	Type
1	a	490	U
1	a	492	C
1	a	493	C
1	a	494	C
1	a	495	U
1	a	497	A
1	a	498	C
1	a	499	G
1	a	500	G
1	a	501	U
1	a	504	C
1	a	505	U
1	a	507	A
1	a	510	A
1	a	512	A
1	a	514	A
1	a	515	G
1	a	517	C
1	a	525	A
1	a	526	C
1	a	530	G
1	a	531	U
1	a	532	G
1	a	533	C
1	a	534	C
1	a	539	G
1	a	542	G
1	a	545	G
1	a	546	U
1	a	547	A
1	a	548	A
1	a	550	A
1	a	551	C
1	a	552	G
1	a	555	G
1	a	556	G
1	a	558	G
1	a	560	C
1	a	561	A
1	a	562	A
1	a	576	U
1	a	577	U

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Mol	Chain	Res	Type
1	a	578	A
1	a	587	A
1	a	588	A
1	a	591	C
1	a	592	G
1	a	594	G
1	a	603	G
1	a	626	C
1	a	627	C
1	a	634	U
1	a	635	C
1	a	636	A
1	a	637	A
1	a	642	G
1	a	644	A
1	a	645	G
1	a	646	G
1	a	647	G
1	a	648	U
1	a	649	C
1	a	664	G
1	a	668	U
1	a	671	G
1	a	672	U
1	a	673	G
1	a	674	C
1	a	676	G
1	a	680	A
1	a	686	G
1	a	701	U
1	a	702	A
1	a	710	A
1	a	723	A
1	a	725	G
1	a	734	C
1	a	736	A
1	a	738	U
1	a	744	A
1	a	749	G
1	a	764	A
1	a	770	G
1	a	782	A

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Mol	Chain	Res	Type
1	a	790	G
1	a	792	A
1	a	809	A
1	a	814	G
1	a	830	A
1	a	831	A
1	a	832	C
1	a	833	G
1	a	836	G
1	a	847	G
1	a	851	G
1	a	858	U
1	a	859	C
1	a	862	C
1	a	867	C
1	a	886	U
1	a	888	A
1	a	892	A
1	a	901	G
1	a	905	A
1	a	930	A
1	a	942	G
1	a	943	G
1	a	950	C
1	a	951	A
1	a	958	G
1	a	964	C
1	a	968	U
1	a	971	U
1	a	975	A
1	a	976	U
1	a	981	A
1	a	982	G
1	a	985	A
1	a	987	G
1	a	988	C
1	a	989	G
1	a	991	A
1	a	992	G
1	a	994	A
1	a	998	U
1	a	999	A

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Mol	Chain	Res	Type
1	a	1000	C
1	a	1005	U
1	a	1008	U
1	a	1009	G
1	a	1011	C
1	a	1018	U
1	a	1019	G
1	a	1020	A
1	a	1021	C
1	a	1022	C
1	a	1025	U
1	a	1029	G
1	a	1030	A
1	a	1031	G
1	a	1035	G
1	a	1038	C
1	a	1040	U
1	a	1041	U
1	a	1042	C
1	a	1043	C
1	a	1044	C
1	a	1045	U
1	a	1046	U
1	a	1047	C
1	a	1049	G
1	a	1050	G
1	a	1052	A
1	a	1053	C
1	a	1054	A
1	a	1055	A
1	a	1060	A
1	a	1061	C
1	a	1069	G
1	a	1070	C
1	a	1080	G
1	a	1081	U
1	a	1082	C
1	a	1094	U
1	a	1095	G
1	a	1101	U
1	a	1102	U
1	a	1110	G

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Mol	Chain	Res	Type
1	a	1111	U
1	a	1117	A
1	a	1124	G
1	a	1140	G
1	a	1141	U
1	a	1147	U
1	a	1148	C
1	a	1149	A
1	a	1152	U
1	a	1154	G
1	a	1155	U
1	a	1156	U
1	a	1157	G
1	a	1161	A
1	a	1169	G
1	a	1174	U
1	a	1175	G
1	a	1176	C
1	a	1183	C
1	a	1184	A
1	a	1189	G
1	a	1198	U
1	a	1199	G
1	a	1201	G
1	a	1208	G
1	a	1211	A
1	a	1212	A
1	a	1227	U
1	a	1228	A
1	a	1229	U
1	a	1230	G
1	a	1241	C
1	a	1243	C
1	a	1256	G
1	a	1272	C
1	a	1275	U
1	a	1276	A
1	a	1284	A
1	a	1289	A
1	a	1295	A
1	a	1297	C
1	a	1300	U

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Mol	Chain	Res	Type
1	a	1301	U
1	a	1302	A
1	a	1303	A
1	a	1305	G
1	a	1312	U
1	a	1314	A
1	a	1317	U
1	a	1318	C
1	a	1320	G
1	a	1324	G
1	a	1327	G
1	a	1332	C
1	a	1335	C
1	a	1337	C
1	a	1350	C
1	a	1351	C
1	a	1355	A
1	a	1362	G
1	a	1368	G
1	a	1374	C
1	a	1379	C
1	a	1393	C
1	a	1396	U
1	a	1398	C
1	a	1413	A
1	a	1416	G
1	a	1434	G
1	a	1438	G
1	a	1441	A
1	a	1448	A
1	a	1455	U
1	a	1457	A
1	a	1461	A
1	a	1466	U
1	a	1467	U
1	a	1468	U
1	a	1500	U
1	a	1503	G
1	a	1508	A
1	a	1509	A
1	a	1510	G
1	a	1513	G

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Mol	Chain	Res	Type
1	a	1515	A
1	a	1518	A
1	a	1519	A
1	a	1522	U
1	a	1523	A
1	a	1545	G
1	a	1546	G
1	a	1547	A
1	a	1549	C
1	a	1550	A
20	A	10	G
20	A	13	U
20	A	14	A
20	A	16	G
20	A	35	U
20	A	62	A
20	A	64	U
20	A	72	A
20	A	76	G
20	A	90	U
20	A	94	U
20	A	97	G
20	A	99	U
20	A	100	A
20	A	102	G
20	A	103	A
20	A	110	G
20	A	116	C
20	A	118	A
20	A	120	U
20	A	131	A
20	A	155	U
20	A	156	U
20	A	163	A
20	A	164	U
20	A	165	A
20	A	166	C
20	A	169	A
20	A	180	G
20	A	181	G
20	A	182	U
20	A	183	A

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Mol	Chain	Res	Type
20	A	184	G
20	A	189	A
20	A	199	A
20	A	202	A
20	A	218	G
20	A	219	A
20	A	224	A
20	A	225	A
20	A	229	A
20	A	231	A
20	A	232	U
20	A	233	U
20	A	235	G
20	A	244	A
20	A	251	G
20	A	254	A
20	A	255	G
20	A	268	A
20	A	279	A
20	A	284	C
20	A	285	U
20	A	288	C
20	A	293	U
20	A	298	U
20	A	300	G
20	A	305	A
20	A	311	A
20	A	312	U
20	A	313	A
20	A	318	A
20	A	319	G
20	A	321	C
20	A	322	U
20	A	332	G
20	A	339	G
20	A	344	G
20	A	367	A
20	A	372	C
20	A	383	A
20	A	389	G
20	A	391	C
20	A	396	C

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Mol	Chain	Res	Type
20	A	399	A
20	A	400	G
20	A	410	G
20	A	421	A
20	A	426	G
20	A	451	G
20	A	452	A
20	A	488	U
20	A	496	C
20	A	507	G
20	A	517	A
20	A	519	A
20	A	521	G
20	A	544	A
20	A	547	U
20	A	548	C
20	A	549	C
20	A	560	U
20	A	561	G
20	A	566	C
20	A	568	A
20	A	569	C
20	A	570	A
20	A	571	A
20	A	572	G
20	A	585	A
20	A	586	A
20	A	588	G
20	A	600	G
20	A	610	G
20	A	612	A
20	A	623	A
20	A	629	G
20	A	640	A
20	A	653	G
20	A	654	A
20	A	655	G
20	A	669	G
20	A	670	A
20	A	673	G
20	A	676	A
20	A	677	G

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Mol	Chain	Res	Type
20	A	684	U
20	A	693	U
20	A	694	G
20	A	696	G
20	A	708	A
20	A	710	A
20	A	711	C
20	A	712	C
20	A	722	G
20	A	726	U
20	A	756	A
20	A	757	A
20	A	759	C
20	A	766	G
20	A	769	G
20	A	770	A
20	A	775	A
20	A	778	C
20	A	787	U
20	A	788	G
20	A	792	A
20	A	805	G
20	A	808	G
20	A	815	G
20	A	816	C
20	A	817	G
20	A	822	A
20	A	823	A
20	A	824	U
20	A	832	G
20	A	833	A
20	A	840	A
20	A	845	G
20	A	846	C
20	A	849	G
20	A	852	C
20	A	867	U
20	A	885	U
20	A	886	U
20	A	887	G
20	A	888	A
20	A	891	A

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Mol	Chain	Res	Type
20	A	900	G
20	A	901	U
20	A	905	G
20	A	906	C
20	A	907	A
20	A	919	A
20	A	920	G
20	A	922	G
20	A	923	G
20	A	925	C
20	A	926	C
20	A	927	A
20	A	928	U
20	A	933	G
20	A	934	G
20	A	939	C
20	A	940	G
20	A	942	A
20	A	943	U
20	A	946	A
20	A	950	A
20	A	951	A
20	A	953	C
20	A	954	U
20	A	960	U
20	A	961	G
20	A	964	A
20	A	966	U
20	A	978	G
20	A	981	A
20	A	982	G
20	A	983	U
20	A	985	A
20	A	986	G
20	A	993	A
20	A	997	A
20	A	999	A
20	A	1001	G
20	A	1006	G
20	A	1014	A
20	A	1016	G
20	A	1023	A

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Mol	Chain	Res	Type
20	A	1036	A
20	A	1048	A
20	A	1049	A
20	A	1051	A
20	A	1052	U
20	A	1053	A
20	A	1057	G
20	A	1061	A
20	A	1062	G
20	A	1063	U
20	A	1064	G
20	A	1065	G
20	A	1066	A
20	A	1073	U
20	A	1085	C
20	A	1086	A
20	A	1087	G
20	A	1093	U
20	A	1096	G
20	A	1097	A
20	A	1098	U
20	A	1100	U
20	A	1101	U
20	A	1103	G
20	A	1104	C
20	A	1105	U
20	A	1106	U
20	A	1107	A
20	A	1108	G
20	A	1109	A
20	A	1110	A
20	A	1111	G
20	A	1113	A
20	A	1114	G
20	A	1116	C
20	A	1117	A
20	A	1118	C
20	A	1120	A
20	A	1122	U
20	A	1123	U
20	A	1124	A
20	A	1125	A

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Mol	Chain	Res	Type
20	A	1127	G
20	A	1128	A
20	A	1129	G
20	A	1131	G
20	A	1132	C
20	A	1134	U
20	A	1135	A
20	A	1136	A
20	A	1137	U
20	A	1138	A
20	A	1139	G
20	A	1140	C
20	A	1141	U
20	A	1142	C
20	A	1143	A
20	A	1144	C
20	A	1146	A
20	A	1147	G
20	A	1148	U
20	A	1149	C
20	A	1151	A
20	A	1152	G
20	A	1157	C
20	A	1167	A
20	A	1168	A
20	A	1170	U
20	A	1171	G
20	A	1172	U
20	A	1174	C
20	A	1175	C
20	A	1179	G
20	A	1181	U
20	A	1182	A
20	A	1188	A
20	A	1190	U
20	A	1209	A
20	A	1212	A
20	A	1215	A
20	A	1216	G
20	A	1217	G
20	A	1218	U
20	A	1249	G

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Mol	Chain	Res	Type
20	A	1257	A
20	A	1275	G
20	A	1277	G
20	A	1287	G
20	A	1290	A
20	A	1292	U
20	A	1293	G
20	A	1294	C
20	A	1308	G
20	A	1309	A
20	A	1310	A
20	A	1311	A
20	A	1336	U
20	A	1337	A
20	A	1338	U
20	A	1349	U
20	A	1357	A
20	A	1365	U
20	A	1366	C
20	A	1375	G
20	A	1377	U
20	A	1388	U
20	A	1394	G
20	A	1396	G
20	A	1401	A
20	A	1404	G
20	A	1407	G
20	A	1411	G
20	A	1415	U
20	A	1420	A
20	A	1422	C
20	A	1428	G
20	A	1431	A
20	A	1432	U
20	A	1436	U
20	A	1439	A
20	A	1443	G
20	A	1446	G
20	A	1447	U
20	A	1448	U
20	A	1449	U
20	A	1450	U

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Mol	Chain	Res	Type
20	A	1451	U
20	A	1452	G
20	A	1453	U
20	A	1455	U
20	A	1456	G
20	A	1457	A
20	A	1461	A
20	A	1462	U
20	A	1463	G
20	A	1465	A
20	A	1469	A
20	A	1470	C
20	A	1471	G
20	A	1475	U
20	A	1488	G
20	A	1489	C
20	A	1492	G
20	A	1493	C
20	A	1494	G
20	A	1495	A
20	A	1497	U
20	A	1500	A
20	A	1501	A
20	A	1502	G
20	A	1503	U
20	A	1504	G
20	A	1505	C
20	A	1508	G
20	A	1509	U
20	A	1510	C
20	A	1519	G
20	A	1521	G
20	A	1525	U
20	A	1535	U
20	A	1536	A
20	A	1539	U
20	A	1548	C
20	A	1551	U
20	A	1552	A
20	A	1559	A
20	A	1560	G
20	A	1566	A

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Mol	Chain	Res	Type
20	A	1567	C
20	A	1568	G
20	A	1573	G
20	A	1576	A
20	A	1577	A
20	A	1579	U
20	A	1584	G
20	A	1585	U
20	A	1586	A
20	A	1589	G
20	A	1601	G
20	A	1604	A
20	A	1605	C
20	A	1606	A
20	A	1608	U
20	A	1612	A
20	A	1613	A
20	A	1615	A
20	A	1623	C
20	A	1627	U
20	A	1629	A
20	A	1630	G
20	A	1631	A
20	A	1632	A
20	A	1633	A
20	A	1634	A
20	A	1646	A
20	A	1650	U
20	A	1651	A
20	A	1653	A
20	A	1673	A
20	A	1674	G
20	A	1677	U
20	A	1689	A
20	A	1690	G
20	A	1691	C
20	A	1717	G
20	A	1718	C
20	A	1737	C
20	A	1741	A
20	A	1746	G
20	A	1756	U

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Mol	Chain	Res	Type
20	A	1757	U
20	A	1770	G
20	A	1776	A
20	A	1777	G
20	A	1778	G
20	A	1782	A
20	A	1784	G
20	A	1787	A
20	A	1790	G
20	A	1795	U
20	A	1798	A
20	A	1814	C
20	A	1815	A
20	A	1823	A
20	A	1829	A
20	A	1830	A
20	A	1840	C
20	A	1841	U
20	A	1842	G
20	A	1843	A
20	A	1872	G
20	A	1882	C
20	A	1886	G
20	A	1896	A
20	A	1913	A
20	A	1917	G
20	A	1920	G
20	A	1927	A
20	A	1928	C
20	A	1943	G
20	A	1944	G
20	A	1948	C
20	A	1952	A
20	A	1969	U
20	A	1970	U
20	A	1978	G
20	A	1979	C
20	A	1980	A
20	A	1981	C
20	A	1984	A
20	A	1985	A
20	A	1986	G

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Mol	Chain	Res	Type
20	A	1989	G
20	A	1990	U
20	A	1996	U
20	A	2005	U
20	A	2006	G
20	A	2007	U
20	A	2010	C
20	A	2030	U
20	A	2035	G
20	A	2036	U
20	A	2037	A
20	A	2039	C
20	A	2044	A
20	A	2045	A
20	A	2046	G
20	A	2047	A
20	A	2048	U
20	A	2057	C
20	A	2066	G
20	A	2069	C
20	A	2070	G
20	A	2074	A
20	A	2075	G
20	A	2076	A
20	A	2082	U
20	A	2083	G
20	A	2114	U
20	A	2115	G
20	A	2125	U
20	A	2126	A
20	A	2127	C
20	A	2129	G
20	A	2131	A
20	A	2132	U
20	A	2133	A
20	A	2134	G
20	A	2139	G
20	A	2140	A
20	A	2141	G
20	A	2144	G
20	A	2145	A
20	A	2146	U

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Mol	Chain	Res	Type
20	A	2147	G
20	A	2148	A
20	A	2154	G
20	A	2158	G
20	A	2159	C
20	A	2160	U
20	A	2162	G
20	A	2163	U
20	A	2173	G
20	A	2174	G
20	A	2175	C
20	A	2176	G
20	A	2179	G
20	A	2180	G
20	A	2182	G
20	A	2183	G
20	A	2187	A
20	A	2189	U
20	A	2196	G
20	A	2201	A
20	A	2206	C
20	A	2207	C
20	A	2212	A
20	A	2213	A
20	A	2217	G
20	A	2218	C
20	A	2224	U
20	A	2225	A
20	A	2227	U
20	A	2239	A
20	A	2252	G
20	A	2253	G
20	A	2280	A
20	A	2281	A
20	A	2282	A
20	A	2293	G
20	A	2296	G
20	A	2297	C
20	A	2301	A
20	A	2302	A
20	A	2318	G
20	A	2319	U

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Mol	Chain	Res	Type
20	A	2323	A
20	A	2327	C
20	A	2333	A
20	A	2334	A
20	A	2336	A
20	A	2337	G
20	A	2339	G
20	A	2341	A
20	A	2348	G
20	A	2349	A
20	A	2350	A
20	A	2361	C
20	A	2364	C
20	A	2367	G
20	A	2372	A
20	A	2379	G
20	A	2390	A
20	A	2393	G
20	A	2397	G
20	A	2398	G
20	A	2399	C
20	A	2404	U
20	A	2405	G
20	A	2406	A
20	A	2417	C
20	A	2420	C
20	A	2433	U
20	A	2436	C
20	A	2437	U
20	A	2439	A
20	A	2441	C
20	A	2442	G
20	A	2443	G
20	A	2445	U
20	A	2455	C
20	A	2462	A
20	A	2473	A
20	A	2488	C
20	A	2489	C
20	A	2508	G
20	A	2517	A
20	A	2518	U

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Mol	Chain	Res	Type
20	A	2519	G
20	A	2521	C
20	A	2534	C
20	A	2548	C
20	A	2549	G
20	A	2557	G
20	A	2561	U
20	A	2563	G
20	A	2570	C
20	A	2571	G
20	A	2580	A
20	A	2581	G
20	A	2586	A
20	A	2587	C
20	A	2596	G
20	A	2599	U
20	A	2600	C
20	A	2616	A
20	A	2622	G
20	A	2623	U
20	A	2624	C
20	A	2627	U
20	A	2628	A
20	A	2629	U
20	A	2631	C
20	A	2650	U
20	A	2660	C
20	A	2675	G
20	A	2677	G
20	A	2696	G
20	A	2703	U
20	A	2722	G
20	A	2727	U
20	A	2728	G
20	A	2735	A
20	A	2740	U
20	A	2746	G
20	A	2747	A
20	A	2749	G
20	A	2753	U
20	A	2762	A
20	A	2766	C

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Mol	Chain	Res	Type
20	A	2771	A
20	A	2778	A
20	A	2779	A
20	A	2780	G
20	A	2792	A
20	A	2793	U
20	A	2804	A
20	A	2805	U
20	A	2812	A
20	A	2813	A
20	A	2814	G
20	A	2831	G
20	A	2835	U
20	A	2836	G
20	A	2841	G
20	A	2844	A
20	A	2845	G
20	A	2846	A
20	A	2850	G
20	A	2854	G
20	A	2858	U
20	A	2868	G
20	A	2870	G
20	A	2878	G
20	A	2883	G
20	A	2891	C
20	A	2895	U
20	A	2897	G
20	A	2902	A
20	A	2904	G
21	B	8	G
21	B	10	G
21	B	13	A
21	B	14	G
21	B	23	A
21	B	24	U
21	B	33	U
21	B	40	C
21	B	42	G
21	B	51	A
21	B	54	U
21	B	55	A

*Continued on next page...*

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Mol	Chain	Res	Type
21	B	64	A
21	B	70	G
21	B	71	A
21	B	81	A
21	B	82	G
21	B	85	U
21	B	86	U
21	B	87	U
21	B	92	U
21	B	94	G
21	B	97	A
21	B	101	U
21	B	102	A
21	B	107	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	179	A
20	A	311	A
20	A	320	U
20	A	386	G
20	A	427	A
20	A	559	G
20	A	654	A
20	A	755	A
20	A	890	A
20	A	960	U
20	A	963	C
20	A	1502	G
20	A	1584	G
20	A	1585	U
20	A	1604	A
20	A	1605	C
20	A	1628	G
20	A	2281	A
20	A	2317	G
20	A	2773	G
21	B	32	U
21	B	101	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	A	2
1	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	928:U	O3'	931:C	P	16.19
1	a	75:U	O3'	96:U	P	13.98
1	A	1579:U	O3'	1583:A	P	9.00



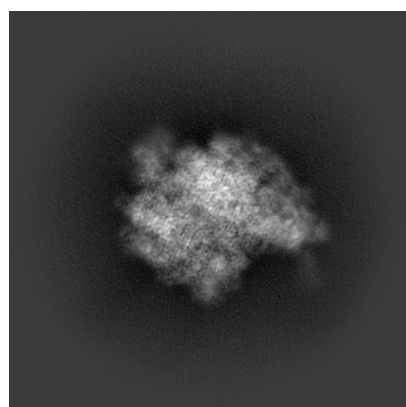
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0660. These allow visual inspection of the internal detail of the map and identification of artifacts.

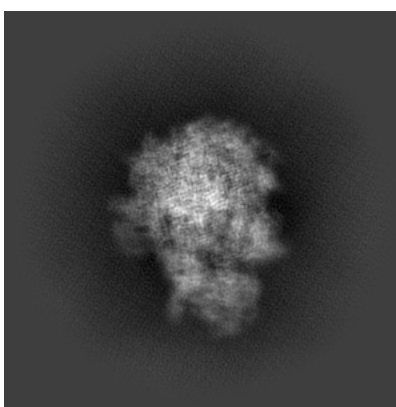
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

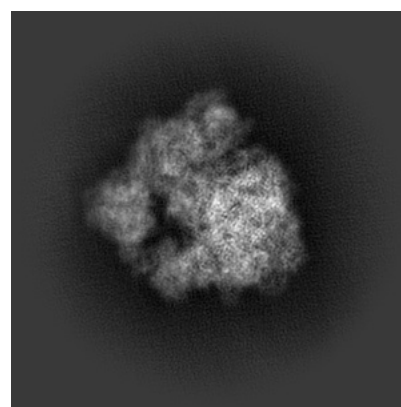
#### 6.1.1 Primary map



X



Y

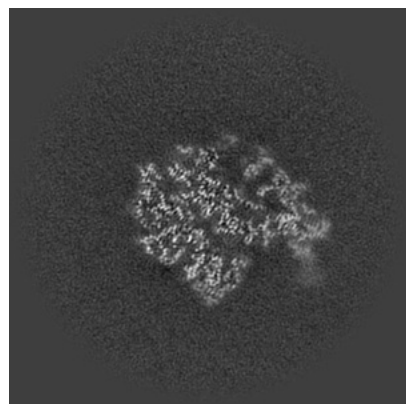


Z

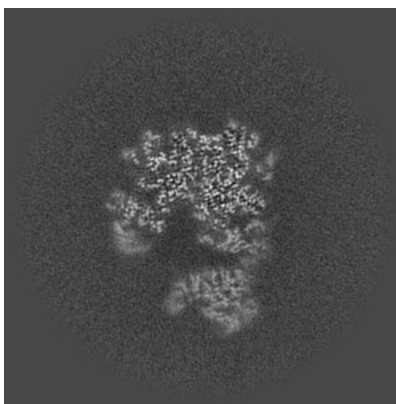
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

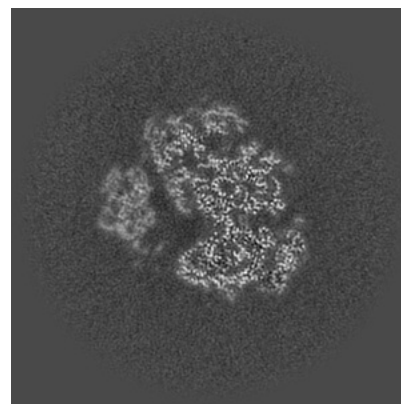
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

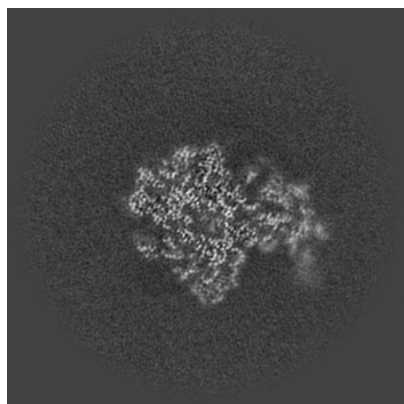


Z Index: 220

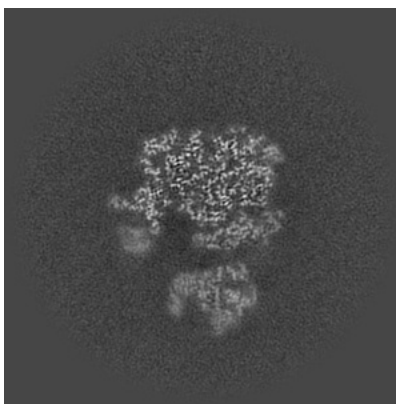
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

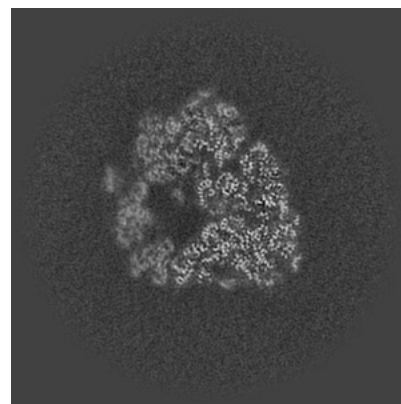
### 6.3.1 Primary map



X Index: 226



Y Index: 231

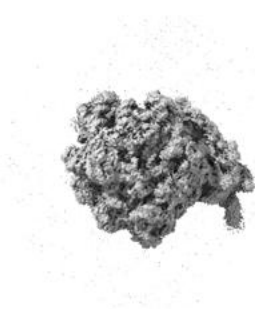


Z Index: 209

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

## 6.4 Orthogonal surface views [i](#)

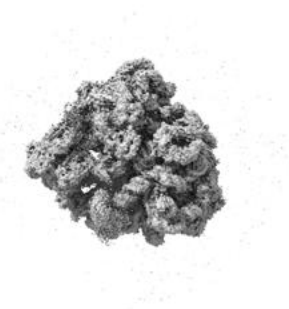
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

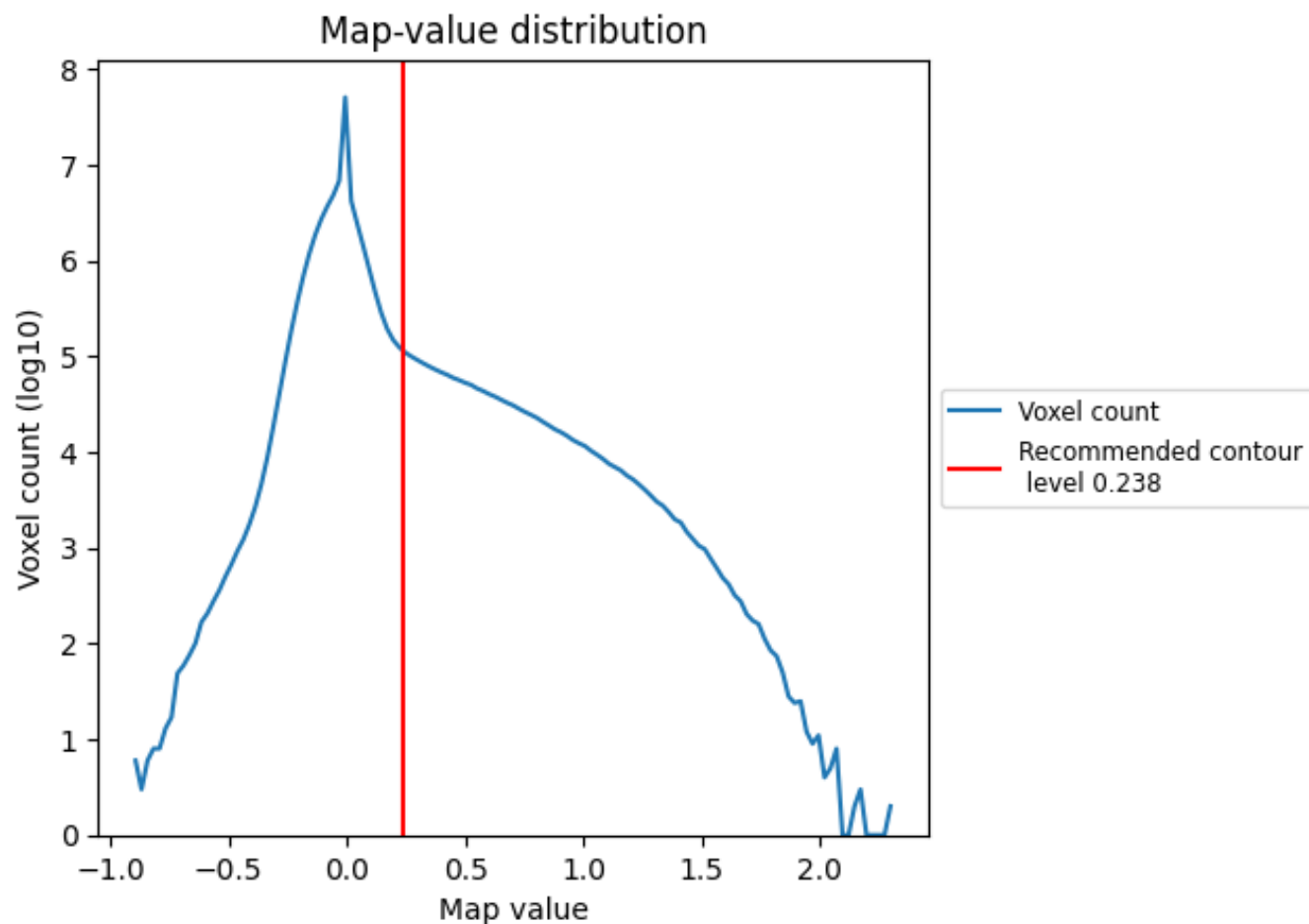
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

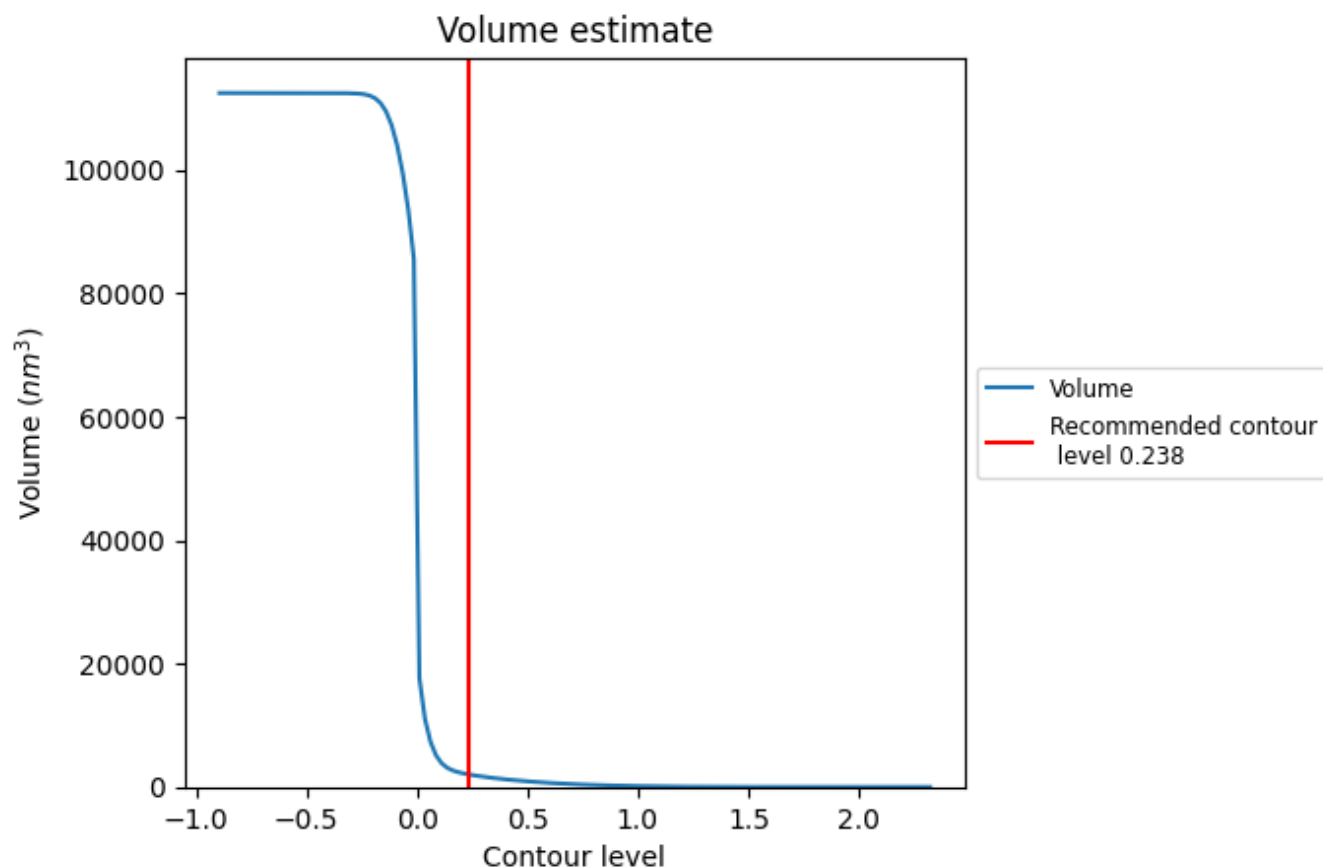
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

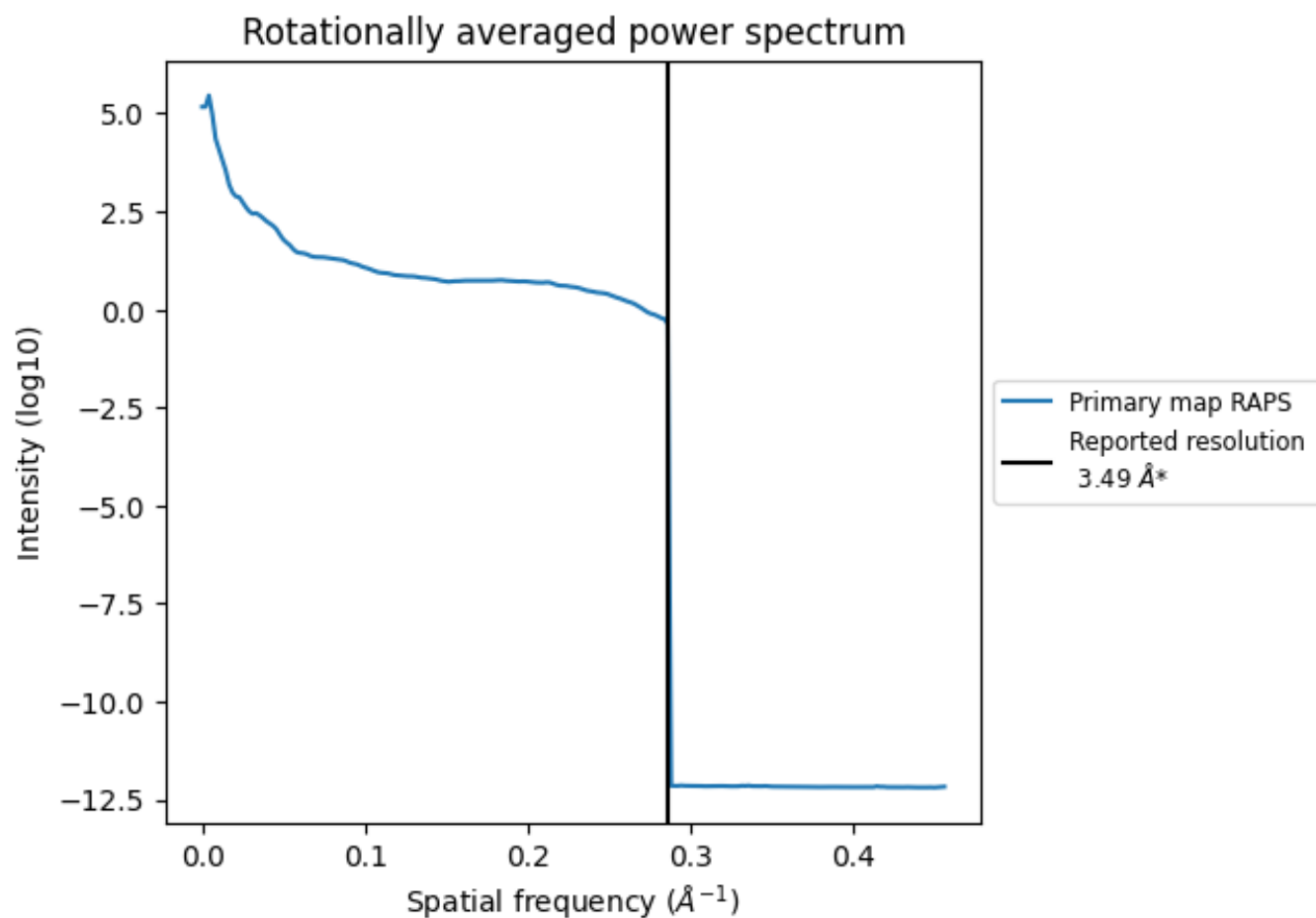
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2006 nm<sup>3</sup>; this corresponds to an approximate mass of 1813 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>

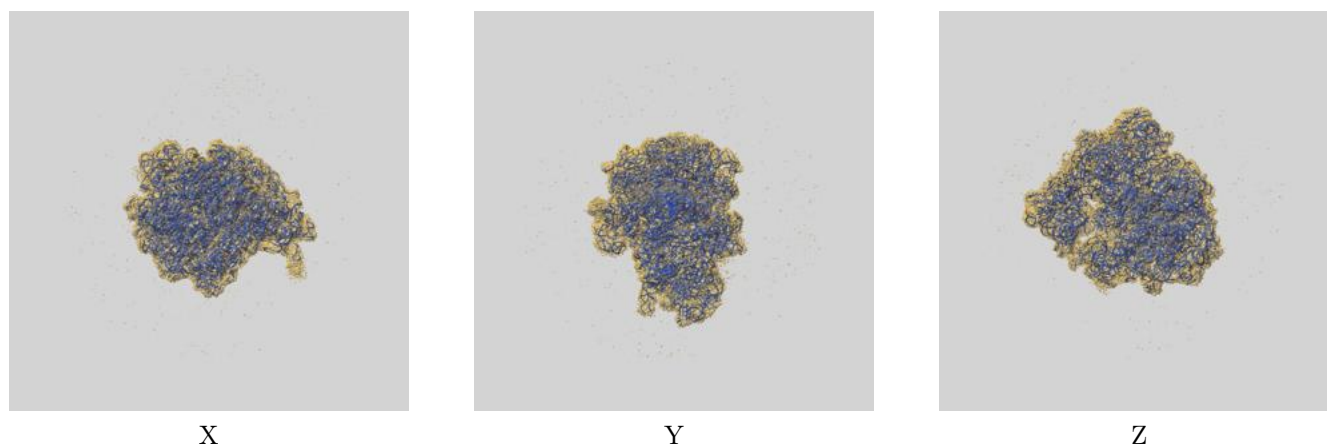
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0660 and PDB model 6O90. Per-residue inclusion information can be found in section [3](#) on page [13](#).

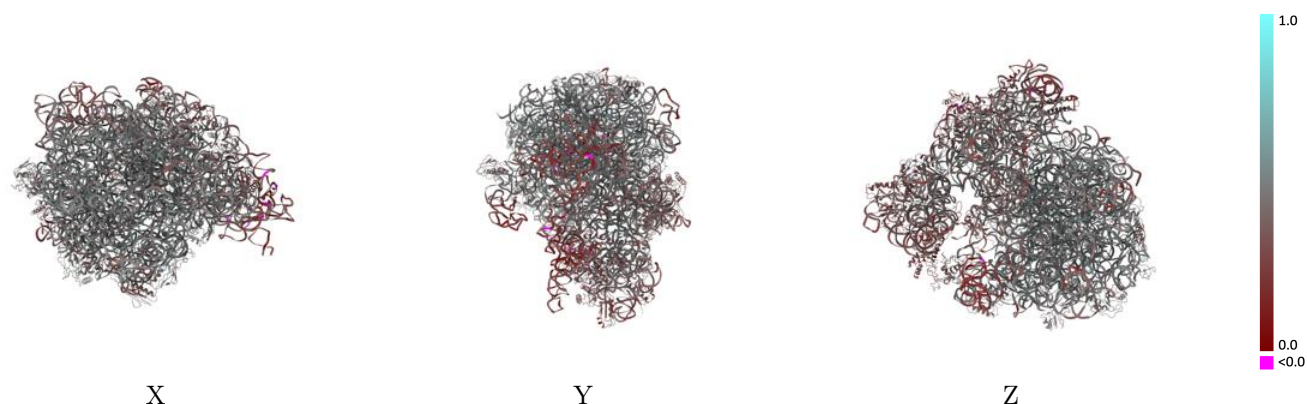
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

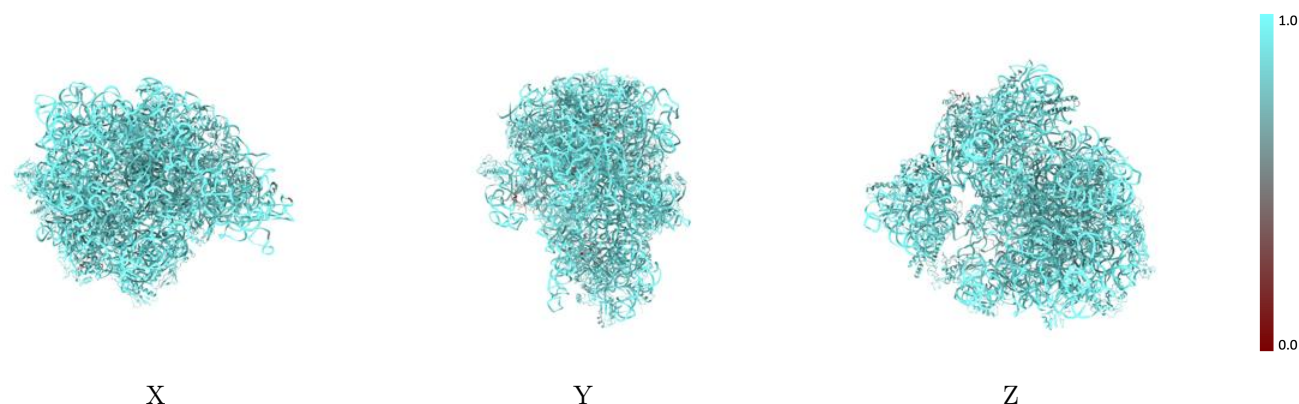


## 9.2 Q-score mapped to coordinate model [i](#)



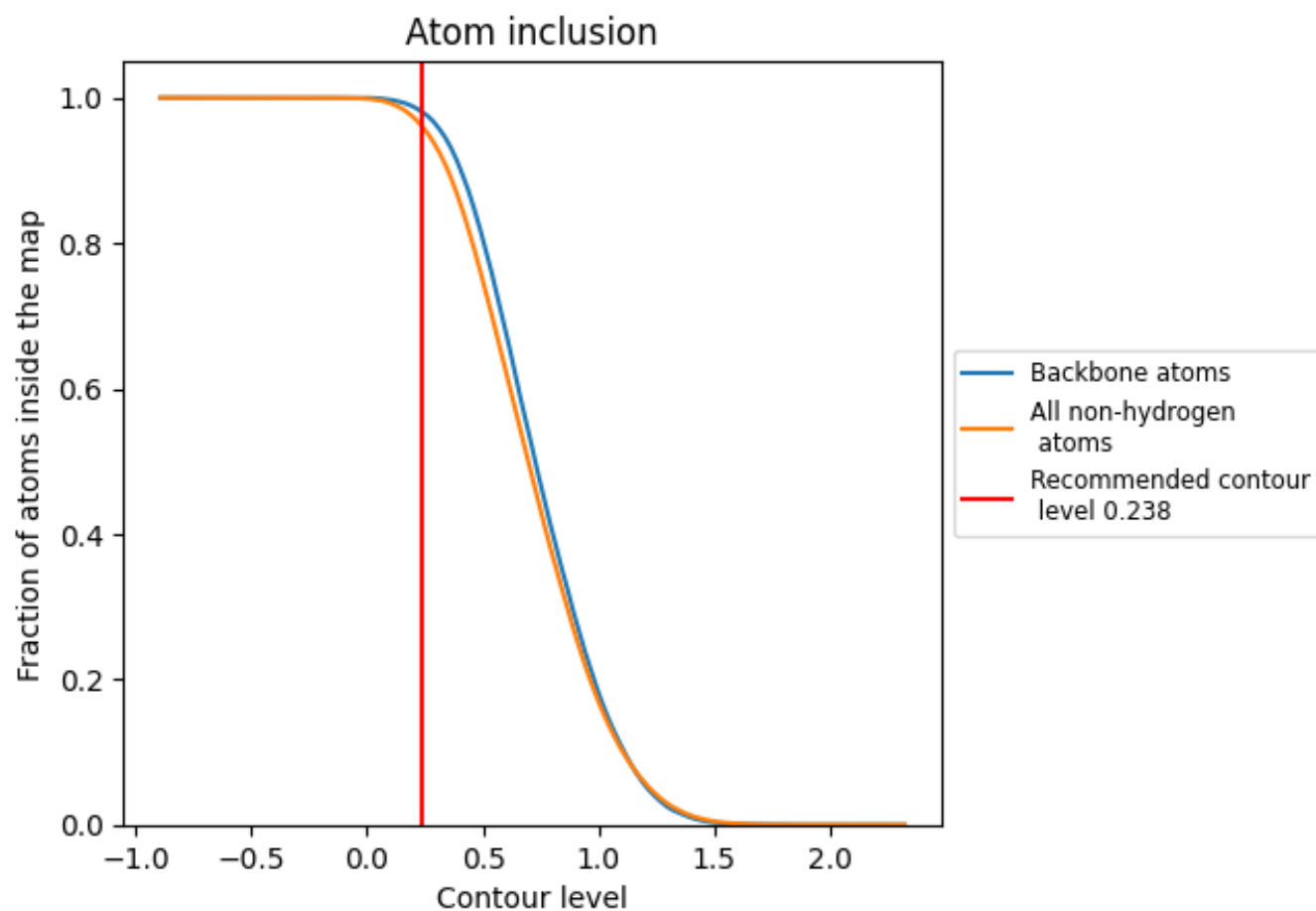
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.238).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ































The table lists the average atom inclusion at the recommended contour level (0.238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9605	 0.4280
0	 0.9182	 0.4660
1	 0.8833	 0.3050
2	 0.9619	 0.4940
3	 0.9059	 0.4700
4	 0.9145	 0.4700
5	 0.9034	 0.4930
6	 0.9524	 0.4820
A	 0.9887	 0.4580
B	 0.9948	 0.4200
C	 0.9300	 0.4780
D	 0.9400	 0.4970
E	 0.9422	 0.4690
F	 0.8763	 0.3670
G	 0.9000	 0.4090
K	 0.9511	 0.4820
L	 0.9175	 0.4930
M	 0.9457	 0.4790
N	 0.8375	 0.4370
O	 0.9364	 0.4670
P	 0.8958	 0.3990
Q	 0.9258	 0.4810
R	 0.9263	 0.4490
S	 0.9161	 0.4630
T	 0.9340	 0.4850
U	 0.9190	 0.4580
V	 0.9001	 0.4450
W	 0.3410	 0.2950
X	 0.9278	 0.4920
Y	 0.9249	 0.4820
Z	 0.9289	 0.4210
a	 0.9911	 0.3940
c	 0.8900	 0.3580
d	 0.7233	 0.2670
e	 0.9009	 0.4220



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Chain	Atom inclusion	Q-score
f	 0.8802	 0.3790
g	 0.8730	 0.3020
h	 0.9222	 0.4100
i	 0.9384	 0.3550
j	 0.8742	 0.3470
k	 0.8785	 0.3970
l	 0.8401	 0.3770
m	 0.8740	 0.2700
n	 0.9432	 0.3970
o	 0.8808	 0.3720
p	 0.9016	 0.3740
q	 0.9035	 0.4190
r	 0.9096	 0.3700
s	 0.8855	 0.3060
t	 0.8164	 0.3340