



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 08:38 PM EST

PDB ID : 6O8Y
EMDB ID : EMD-0658
Title : Cryo-EM image reconstruction of the 70S Ribosome *Enterococcus faecalis* Class03
Authors : Jogl, G.; Khayat, R.
Deposited on : 2019-03-12
Resolution : 4.14 Å (reported)
Based on initial models : 5LI0, 4YBB

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
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

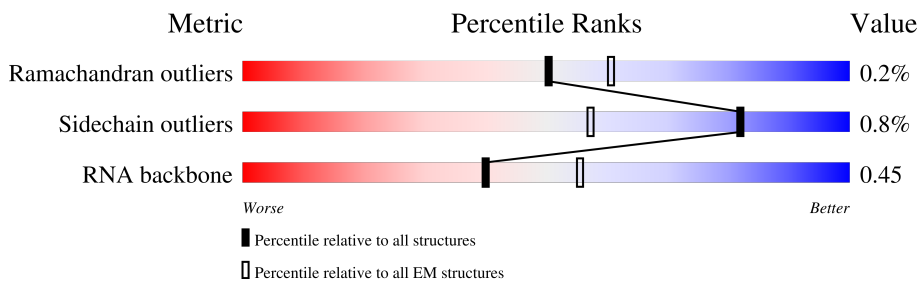
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.14 Å.

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



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

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

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

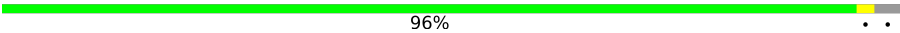
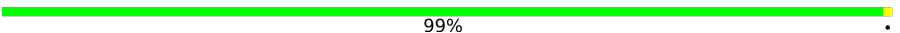
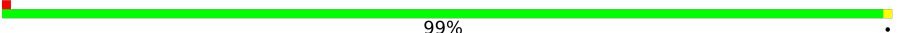
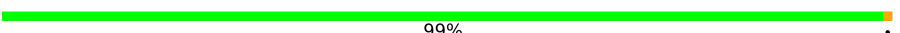
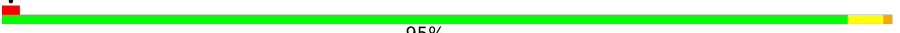





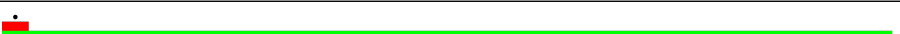


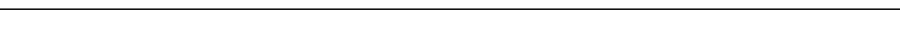
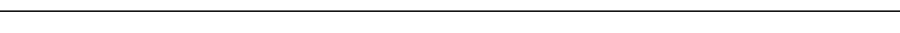
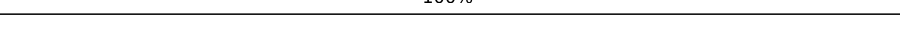
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Mol	Chain	Length	Quality of chain
9	j	99	
10	k	117	
11	l	136	
12	m	112	
13	n	60	
14	o	88	
15	p	89	
16	q	83	
17	r	66	
18	s	78	
19	t	81	
20	A	2903	
21	B	116	
22	C	275	
23	D	207	
24	E	206	
25	F	177	
26	G	176	
27	K	145	
28	L	122	
29	M	146	
30	N	141	
31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

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Mol	Chain	Length	Quality of chain
34	R	118	 96% . .
35	S	102	 99% .
36	T	112	 99% .
37	U	89	 99% .
38	V	101	 95% . .
39	W	94	 63% 98% .
40	X	76	 99% .
41	Y	54	 96% .
42	Z	61	 100%
43	0	58	 100%
44	1	60	 100%
45	2	56	 98% .
46	3	49	 100%
47	4	44	 95% 5%
48	5	64	 100%
49	6	38	 100%

2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 138210 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	2897	Total	C	N	O	P	0	0
			62176	27750	11434	20095	2897		

- Molecule 21 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	116	Total	C	N	O	P	0	0
			2478	1105	444	813	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
			1578	993	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
			1572	982	290	298	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	886	239	260	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	841	244	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	709	216	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	114	Total	C	N	O	0	0
			924	582	185	157		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R	115	Total	C	N	O	S	0	1
			913	578	175	156	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	458	126	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	134	140	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
			572	351	109	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
			424	265	85	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
			435	271	81	82	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	60	Total	C	N	O	S	0	0
			475	302	74	97	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
			419	253	86	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
			373	226	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
			304	188	66	44	6		

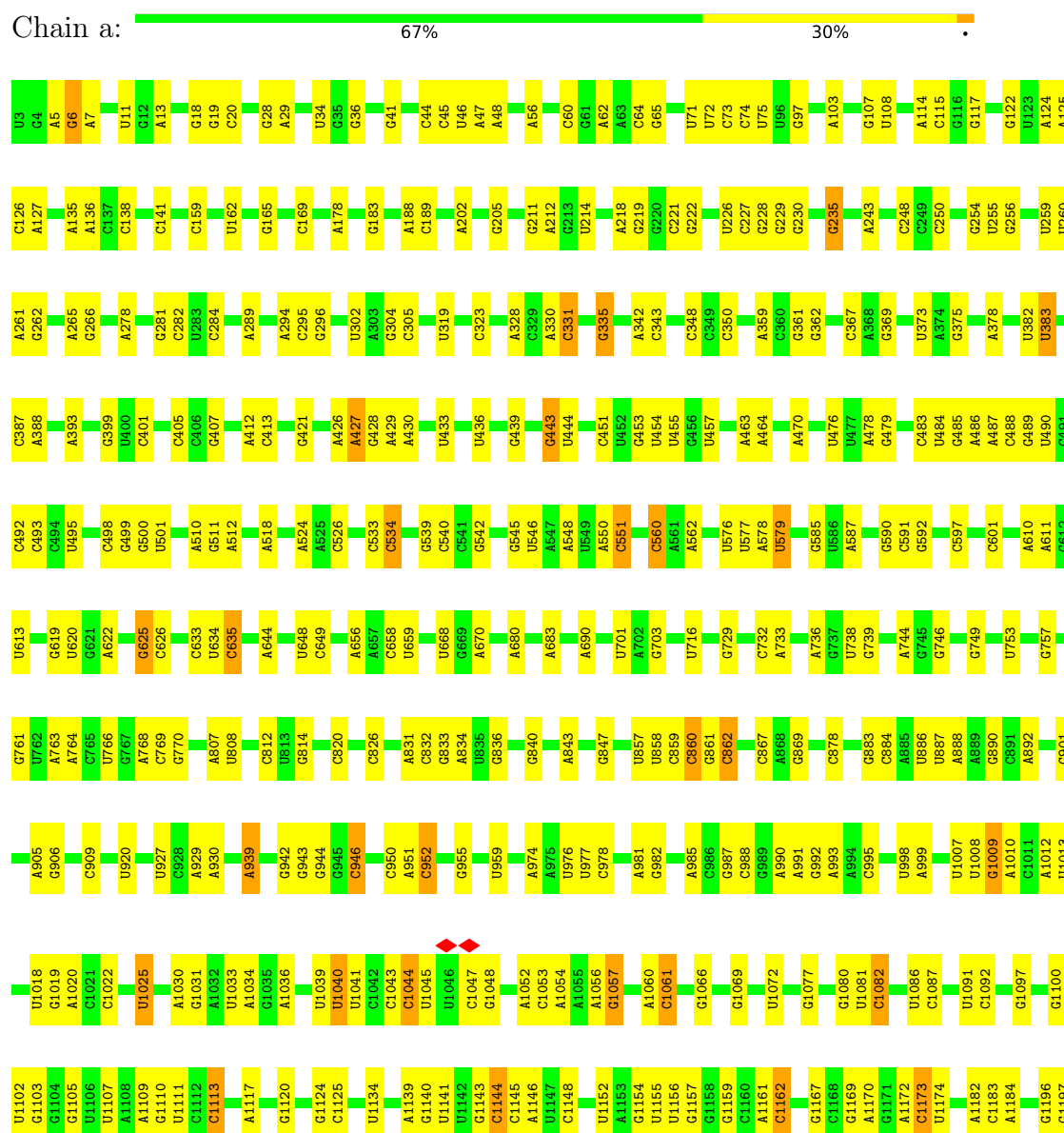
- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
50	n	1	Total	Zn	0
			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

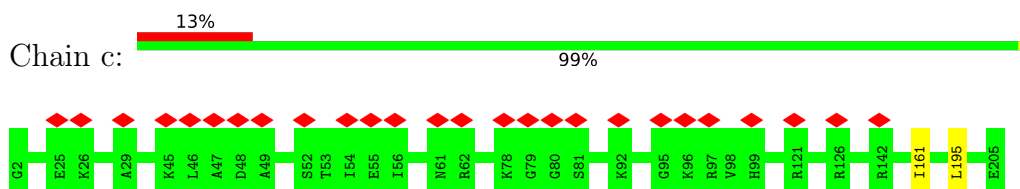
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

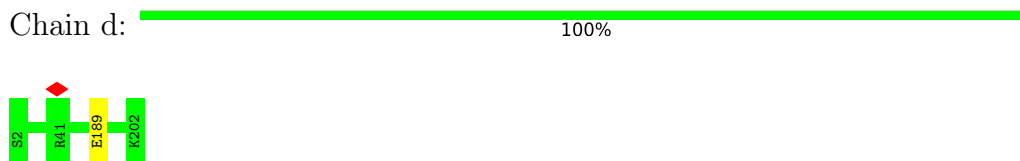




- Molecule 2: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S4

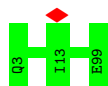


- Molecule 4: 30S ribosomal protein S5

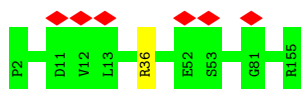


There are no outlier residues recorded for this chain.

- Molecule 5: 30S ribosomal protein S6

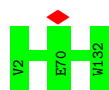


- Molecule 6: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S8

Chain h:  100%



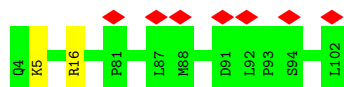
- Molecule 8: 30S ribosomal protein S9

Chain i:  98%



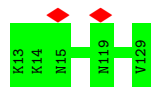
- Molecule 9: 30S ribosomal protein S10

Chain j:  98%



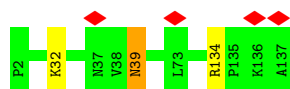
- Molecule 10: 30S ribosomal protein S11

Chain k:  100%



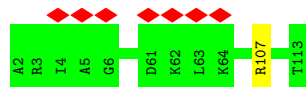
- Molecule 11: 30S ribosomal protein S12

Chain l:  98%



- Molecule 12: 30S ribosomal protein S13

Chain m:  99%



- Molecule 13: 30S ribosomal protein S14 type Z

Chain n:  98%



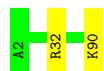
- Molecule 14: 30S ribosomal protein S15

Chain o:  98%



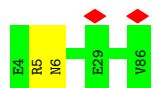
- Molecule 15: 30S ribosomal protein S16

Chain p:  98%

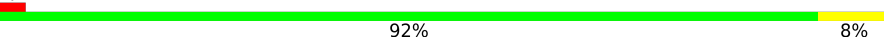


- Molecule 16: 30S ribosomal protein S17

Chain q:  98%



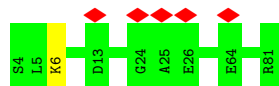
- Molecule 17: 30S ribosomal protein S18

Chain r:  92% 8%



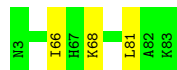
- Molecule 18: 30S ribosomal protein S19

Chain s:  6% 99%



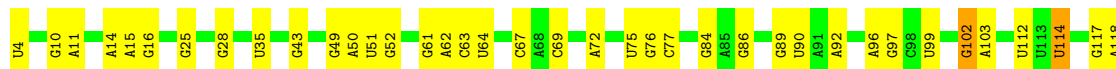
- Molecule 19: 30S ribosomal protein S20

Chain t:  96%

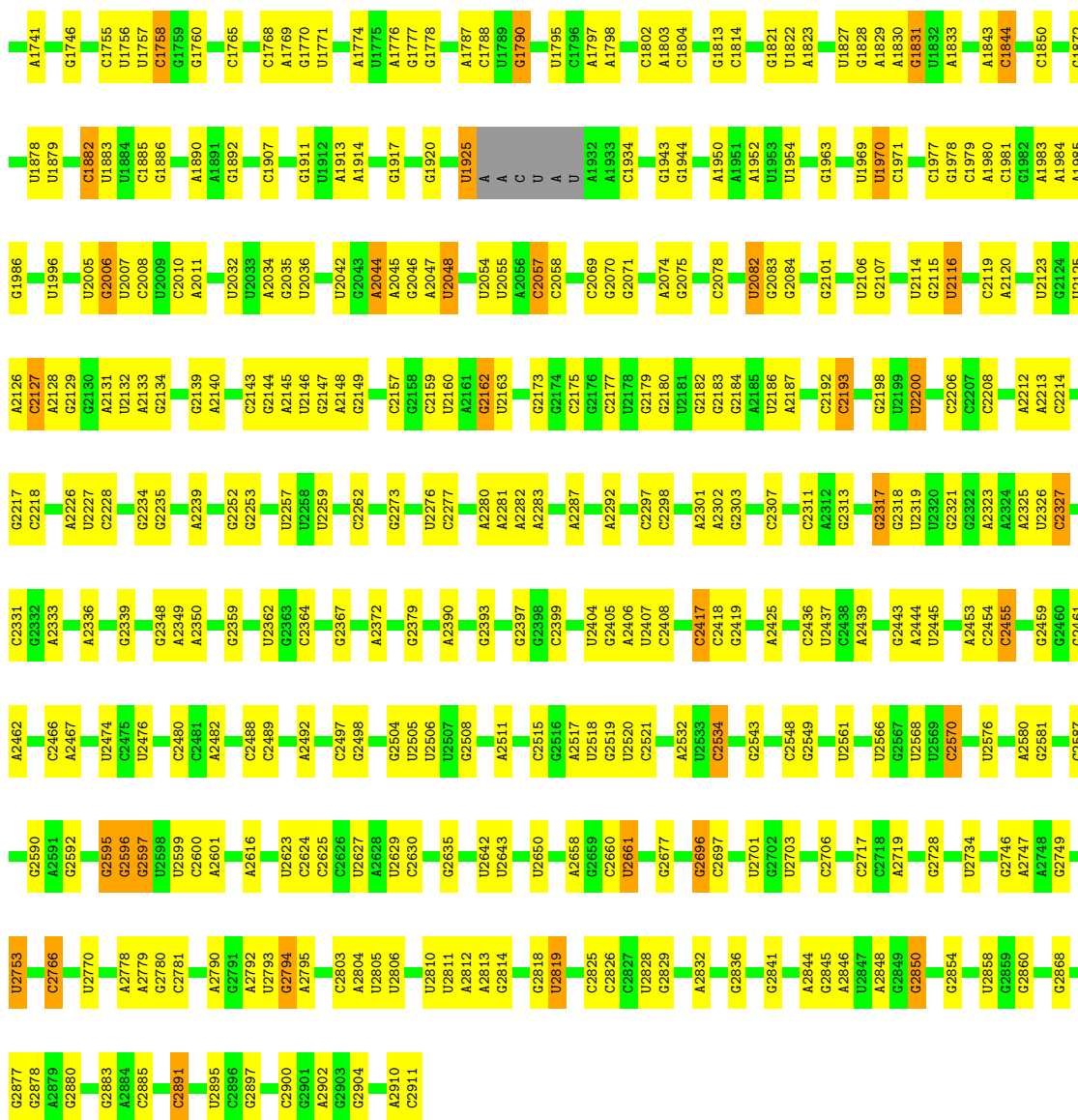


- Molecule 20: 23S rRNA

Chain A:  66% 30%

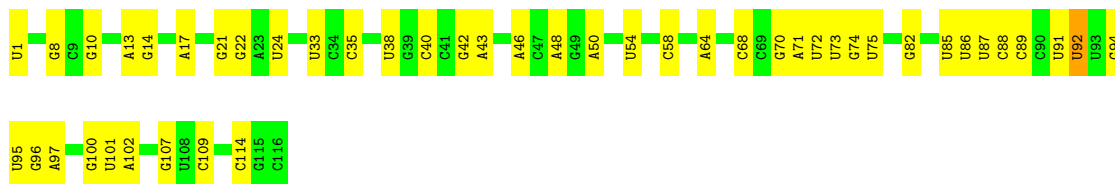


A1612	A1613	G1614	A1615	U1622	C1623	A1624	A1625	G1626	A1629	G1630	A1631	A1632	A1633	A1634	C1638	C1647	G1648	G1649	U1650	A1651	A1652	A1653	A1665	G1674	U1677	C1680	A1683	A1689	G1690	C1691	C1695	G1696	A1697	C1703	A1708	A1711	G1717	C1718	A1719	A1720	U1723	G1730										
G1519	A1520	G1521	U1525	A1530	G1531	A1532	G1533	A1536	U1539	G1540	C1541	A1545	C1548	U1551	A1552	A1559	G1560	U1561	A1566	C1567	G1568	G1569	A1572	G1573	A1574	G1575	A1576	A1577	G1584	U1585	A1586	G1587	G1588	A1589	A1590	G1592	U1593	A1599	C1600	G1601	A1604	C1605	A1606									
U1433	C1434	U1435	U1436	A1439	G1443	U1444	U1445	G1446	U1447	U1448	U1449	U1450	U1451	G1452	U1453	U1454	U1455	G1456	A1457	G1458	A1461	U1462	G1463	A1469	G1470	C1471	C1472	U1475	C1479	G1488	C1489	A1490	U1491	G1492	C1493	G1494	A1495	U1496	U1497	A1500	A1501	G1502	U1503	G1504	U1507	G1508	U1509	C1510	C1511	A1512		
U1327	G1335	U1336	A1337	U1347	U1348	U1349	C1350	G1359	G1360	C1363	G1364	U1365	C1366	C1367	G1368	C1369	G1373	U1376	U1377	A1378	C1386	C1393	G1396	G1397	A1401	G1404	U1408	G1410	G1411	A1414	U1415	G1416	A1418	C1419	A1420	A1421	U1427	G1428	A1429	U1430	U1431	U1432										
C1193	G1194	A1195	U1196	C1197	C1198	U1199	A1209	C1210	U1211	A1212	U1213	A1214	A1215	G1216	G1217	U1218	G1219	U1220	U1236	U1247	U1248	A1257	U1258	G1265	A1266	U1271	G1272	G1273	A1274	G1275	G1276	G1277	A1284	G1285	A1290	U1291	U1292	G1293	C1294	A1302	G1303	U1304	G1308	A1309	A1310	A1311	G1317					
A1113	G1114	C1115	A1116	A1117	C1118	C1119	A1120	U1121	U1122	U1123	A1124	A1125	A1126	G1127	A1128	G1129	U1130	G1131	C1132	A1135	A1136	U1137	A1138	G1139	U1140	U1141	A1143	C1144	U1145	A1146	G1147	U1148	A1151	G1152	U1153	G1154	A1155	C1156	G1162	A1166	A1167	A1168	G1171	U1172	A1173	C1174	C1175	G1176	G1179	C1180	U1181	A1182
G1016	A1020	A1023	U1024	C1025	G1029	A1036	U1039	C1047	A1048	A1049	A1050	A1051	U1052	A1053	A1060	G1062	U1063	A1066	U1073	U1081	A1084	A1085	A1086	G1087	A1088	C1089	C1092	U1093	A1094	G1095	G1096	A1097	U1098	G1099	U1100	U1101	G1102	G1103	C1104	U1105	G1108	A1109	A1110	G1111	C1112							
A919	G920	C925	C926	A927	U928	C931	G932	G933	G934	U935	U936	A937	C938	C939	A840	A842	G845	C846	U847	G848	C849	U850	U851	U853	U867	U868	A869	G870	U874	U886	G887	A888	G889	A890	A891	U892	G900	U901	A904	G905	C906	A907	G910	U911	U912	U913	G914	C917	U918			
A948	U949	A950	A951	C953	C956	G957	A958	U960	G961	C962	C963	A964	U965	U966	G979	G980	A985	G986	G992	A993	G996	U997	U998	A999	A1000	G1001	A1014	A1015																								
A822	A823	U824	U825	A828	A829	A830	G832	A833	A834	U837	A840	G841	A842	G845	C846	U847	G848	C849	U850	U851	U853	U867	U868	A869	G870	U874	U886	G887	A888	G889	A890	A891	U892	G900	U901	A904	G905	C906	A907	G910	U911	U912	U913	G914	C917	U918						
A710	C711	C712	G713	G714	A715	A716	U721	G722	A725	U726	C730	A739	G740	G741	U742	A756	G757	A758	G759	A762	G766	G767	G768	G769	A770	C771	C772	G773	A774	A775	C776	G785	U786	U787	A791	A792	A801	U802	G803	A804	G805	G808	A814	U815	C816	G817						
A585	A586	U587	G588	G592	G595	G600	C601	C602	U605	U606	U608	A609	G610	A611	A612	C621	C622	A623	C638	G639	A640	G641	G642	U643	U644	C649	G653	C654	A654	G655	C657	G673	G674	G675	A676	G677	A682	A683	U684	U683	G694	A695	A698	A708	G709							
A487	U488	A489	A494	C495	C496	U499	U504	G505	A506	G507	G508	G509	A517	A518	A519	G520	A523	C527	G533	G534	G535	U543	A544	U547	C548	G549	U550	G551	A554	C555	G561	A565	C566	A567	A568	C569	A570	A571	U572	U573	C574	A575	A576	U580								
G243	A244	G250	C251	G252	G253	A254	G255	A258	A268	G269	C270	C271	C272	A279	C284	U285	U286	G287	C288	U293	G294	G297	U298	U299	G300	G310	A311	U312	A313	G316	U317	A318	C321	U322	G323	U324	A325	A326	G332	G339	G344	U325	G345	A346	A347	C352						
C353	G354	A359	A367	A368	A369	G370	G375	A383	A390	C391	A392	A393	C394	C395	A396	A399	G403	G404	G410	A414	A421	A422	A423	A424	G426	A427	A430	U433	G446	A451	C454	A458	A462	U471	G475	C476	C484															
A119	U120	G121	A131	G134	A134	U137	U140	A143	A151	U155	U156	A162	A163	U164	A165	C166	A167	U168	A169	G170	C171	G297	U298	U299	G300	G310	A311	U312	A313	G316	U317	A318	C321	U322	G323	U324	A325	A326	G332	A346	A347	C352										



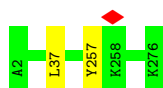
• Molecule 21: 5S rRNA

Chain B: 60% 39%



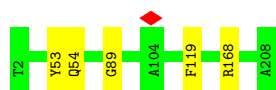
• Molecule 22: 50S ribosomal protein L2

Chain C: 99%



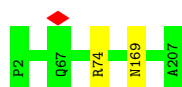
- Molecule 23: 50S ribosomal protein L3

Chain D:  98% .



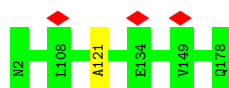
- Molecule 24: 50S ribosomal protein L4

Chain E:  99% .



- Molecule 25: 50S ribosomal protein L5

Chain F:  99% .



- Molecule 26: 50S ribosomal protein L6

Chain G:  99% ..



- Molecule 27: 50S ribosomal protein L13

Chain K:  100%

There are no outlier residues recorded for this chain.

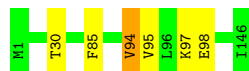
- Molecule 28: 50S ribosomal protein L14

Chain L:  100%

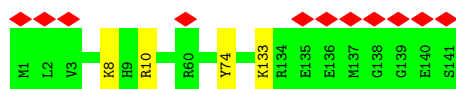
There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L15

Chain M:  96% ..



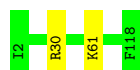
- Molecule 30: 50S ribosomal protein L16



- Molecule 31: 50S ribosomal protein L17



- Molecule 32: 50S ribosomal protein L18



- Molecule 33: 50S ribosomal protein L19

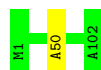


There are no outlier residues recorded for this chain.

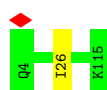
- Molecule 34: 50S ribosomal protein L20



- Molecule 35: 50S ribosomal protein L21



- Molecule 36: 50S ribosomal protein L22



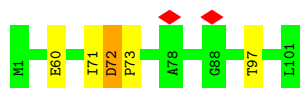
- Molecule 37: 50S ribosomal protein L23

Chain U:  99%



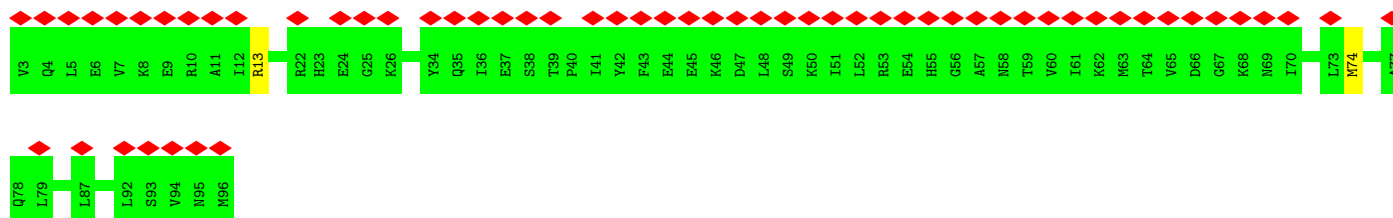
- Molecule 38: 50S ribosomal protein L24

Chain V:  95%



- Molecule 39: 50S ribosomal protein L25

Chain W:  63%
98%



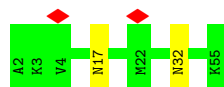
- Molecule 40: 50S ribosomal protein L27

Chain X:  99%



- Molecule 41: 50S ribosomal protein L28

Chain Y:  96%



- Molecule 42: 50S ribosomal protein L29

Chain Z:  100%

There are no outlier residues recorded for this chain.

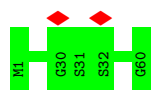
- Molecule 43: 50S ribosomal protein L30

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L31 type B

Chain 1:  100%



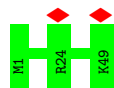
- Molecule 45: 50S ribosomal protein L32

Chain 2:  98%



- Molecule 46: 50S ribosomal protein L33

Chain 3:  100%



- Molecule 47: 50S ribosomal protein L34

Chain 4:  95% 5%



- Molecule 48: 50S ribosomal protein L35

Chain 5:  100%

There are no outlier residues recorded for this chain.

- 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	18979	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	1.406	Depositor
Minimum map value	-0.456	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.078	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	0.68	1/36657 (0.0%)	1.20	226/57173 (0.4%)
2	c	0.29	0/1635	0.58	1/2197 (0.0%)
3	d	0.36	0/1650	0.61	0/2217
4	e	0.34	0/1217	0.58	0/1641
5	f	0.38	0/807	0.55	0/1087
6	g	0.29	0/1249	0.51	0/1682
7	h	0.40	0/1054	0.59	0/1417
8	i	0.31	0/1003	0.57	0/1343
9	j	0.29	0/812	0.64	0/1093
10	k	0.34	0/878	0.61	0/1185
11	l	0.35	0/1082	0.65	1/1453 (0.1%)
12	m	0.30	0/890	0.57	0/1195
13	n	0.29	0/504	0.51	0/669
14	o	0.37	0/751	0.56	0/1001
15	p	0.42	0/720	0.62	0/966
16	q	0.38	0/689	0.67	0/920
17	r	0.34	0/544	0.61	0/728
18	s	0.33	0/650	0.58	0/872
19	t	0.31	0/612	0.56	0/818
20	A	0.85	6/69635 (0.0%)	1.25	478/108600 (0.4%)
21	B	0.79	1/2769 (0.0%)	1.23	16/4311 (0.4%)
22	C	0.44	0/2147	0.67	1/2886 (0.0%)
23	D	0.45	0/1598	0.70	0/2144
24	E	0.43	0/1593	0.59	0/2154
25	F	0.35	0/1408	0.58	0/1891
26	G	0.37	0/1362	0.66	0/1833
27	K	0.44	0/1149	0.65	0/1552
28	L	0.45	0/929	0.66	0/1247
29	M	0.40	0/1102	0.72	0/1468
30	N	0.45	0/1139	0.69	0/1515
31	O	0.43	0/986	0.75	2/1321 (0.2%)
32	P	0.39	0/907	0.62	0/1214

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Q	0.46	0/938	0.67	0/1262
34	R	0.46	0/922	0.67	0/1223
35	S	0.42	0/794	0.61	0/1065
36	T	0.41	0/858	0.63	0/1157
37	U	0.43	0/725	0.72	0/967
38	V	0.39	0/772	0.72	2/1035 (0.2%)
39	W	0.31	0/767	0.63	0/1029
40	X	0.47	0/578	0.62	0/773
41	Y	0.36	0/430	0.57	0/572
42	Z	0.35	0/505	0.56	0/672
43	0	0.39	0/437	0.68	0/589
44	1	0.34	0/488	0.62	0/663
45	2	0.47	0/436	0.59	0/578
46	3	0.34	0/423	0.57	0/563
47	4	0.42	0/375	0.64	0/487
48	5	0.37	0/528	0.60	0/689
49	6	0.41	0/309	0.58	0/409
All	All	0.71	8/150413 (0.0%)	1.12	727/225526 (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
2	c	0	1
3	d	0	1
17	r	0	2
19	t	0	2
23	D	0	2
25	F	0	1
26	G	0	2
29	M	0	4
30	N	0	2
31	O	0	1
32	P	0	2
34	R	0	1
35	S	0	1
36	T	0	1
37	U	0	1
38	V	0	2
39	W	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	X	0	1
47	4	0	2
All	All	0	30

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1	U	OP3-P	-10.80	1.48	1.61
1	a	243	A	N9-C4	-6.63	1.33	1.37
20	A	1689	A	N9-C4	6.58	1.41	1.37
20	A	1414	A	N9-C4	-5.81	1.34	1.37
20	A	422	A	N9-C4	-5.79	1.34	1.37
20	A	828	A	N9-C4	-5.74	1.34	1.37
20	A	1146	A	N9-C4	5.66	1.41	1.37
20	A	1572	A	N9-C4	-5.27	1.34	1.37

All (727) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1335	C	N1-C2-O2	13.66	127.09	118.90
20	A	1092	C	N1-C2-O2	12.19	126.22	118.90
20	A	1551	U	C2-N1-C1'	12.15	132.28	117.70
20	A	1349	U	N3-C2-O2	-11.56	114.11	122.20
20	A	1551	U	N1-C2-O2	11.44	130.81	122.80
1	a	995	C	C2-N1-C1'	11.38	131.32	118.80
20	A	495	C	N1-C2-O2	10.99	125.50	118.90
1	a	995	C	N1-C2-O2	10.70	125.32	118.90
20	A	1130	U	C2-N1-C1'	10.62	130.44	117.70
1	a	769	C	C2-N1-C1'	10.29	130.12	118.80
20	A	1551	U	N3-C2-O2	-10.23	115.04	122.20
20	A	1199	U	N3-C2-O2	-10.11	115.12	122.20
1	a	1335	C	N3-C2-O2	-10.05	114.87	121.90
20	A	1130	U	N3-C2-O2	-9.97	115.22	122.20
1	a	1446	C	N1-C2-O2	9.69	124.72	118.90
20	A	1349	U	N1-C2-O2	9.58	129.51	122.80
1	a	1306	C	C2-N1-C1'	9.56	129.32	118.80
1	a	1082	C	N1-C2-O2	9.55	124.63	118.90
1	a	141	C	N1-C2-O2	9.54	124.63	118.90
20	A	2048	U	C2-N1-C1'	9.48	129.07	117.70
20	A	1092	C	C2-N1-C1'	9.43	129.17	118.80
20	A	1453	U	C2-N1-C1'	9.36	128.94	117.70
20	A	913	U	N3-C2-O2	-9.32	115.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	68	C	N1-C2-O2	9.32	124.49	118.90
21	B	68	C	C2-N1-C1'	9.20	128.92	118.80
1	a	1335	C	C2-N1-C1'	9.18	128.90	118.80
20	A	1092	C	N3-C2-O2	-9.12	115.52	121.90
20	A	1130	U	N1-C2-O2	9.10	129.17	122.80
20	A	644	U	N3-C2-O2	-9.06	115.86	122.20
1	a	649	C	C6-N1-C2	-9.04	116.68	120.30
20	A	1367	C	N3-C2-O2	-9.04	115.57	121.90
1	a	634	U	C2-N1-C1'	8.91	128.39	117.70
1	a	1082	C	C2-N1-C1'	8.91	128.60	118.80
1	a	995	C	N3-C2-O2	-8.88	115.69	121.90
20	A	2007	U	N1-C2-O2	8.80	128.96	122.80
20	A	1349	U	C2-N1-C1'	8.76	128.21	117.70
1	a	995	C	C6-N1-C2	-8.75	116.80	120.30
20	A	2826	C	C2-N1-C1'	8.68	128.34	118.80
20	A	1448	U	N1-C2-O2	8.60	128.82	122.80
20	A	2082	U	C2-N1-C1'	8.60	128.02	117.70
20	A	2825	C	N1-C2-O2	8.60	124.06	118.90
20	A	913	U	N1-C2-O2	8.54	128.78	122.80
20	A	2007	U	N3-C2-O2	-8.47	116.27	122.20
20	A	1104	C	N1-C2-O2	8.47	123.98	118.90
1	a	1465	U	N1-C2-O2	8.45	128.72	122.80
1	a	952	C	C6-N1-C2	-8.43	116.93	120.30
20	A	422	A	C2-N3-C4	-8.43	106.39	110.60
1	a	73	C	N1-C2-O2	8.40	123.94	118.90
20	A	2488	C	N1-C2-O2	8.38	123.93	118.90
20	A	495	C	N3-C2-O2	-8.31	116.08	121.90
20	A	1199	U	N1-C2-O2	8.29	128.60	122.80
20	A	1551	U	C6-N1-C1'	-8.25	109.65	121.20
1	a	1306	C	N1-C2-O2	8.23	123.84	118.90
1	a	1482	C	N3-C2-O2	-8.23	116.14	121.90
20	A	2506	U	N3-C2-O2	-8.21	116.45	122.20
20	A	1360	G	N3-C4-N9	-8.19	121.09	126.00
20	A	1804	C	C6-N1-C2	-8.15	117.04	120.30
1	a	1113	C	N3-C2-O2	-8.00	116.30	121.90
20	A	1092	C	C6-N1-C2	-8.00	117.10	120.30
1	a	946	C	C2-N1-C1'	7.99	127.58	118.80
1	a	634	U	N1-C2-O2	7.96	128.38	122.80
1	a	1152	U	N1-C2-O2	7.94	128.36	122.80
20	A	433	U	N1-C2-O2	7.93	128.35	122.80
20	A	607	G	C4-N9-C1'	7.91	136.78	126.50
20	A	935	U	C2-N1-C1'	7.89	127.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	730	C	C6-N1-C2	-7.87	117.15	120.30
20	A	1115	C	N3-C2-O2	-7.85	116.41	121.90
20	A	1092	C	C5-C6-N1	7.82	124.91	121.00
20	A	2006	G	O4'-C1'-N9	-7.81	101.95	108.20
20	A	2825	C	N3-C2-O2	-7.81	116.43	121.90
1	a	1152	U	C2-N1-C1'	7.80	127.06	117.70
20	A	1647	C	C6-N1-C2	-7.79	117.19	120.30
20	A	1758	C	C2-N1-C1'	7.79	127.37	118.80
20	A	1213	U	N3-C2-O2	-7.79	116.75	122.20
20	A	1758	C	N1-C2-O2	7.78	123.57	118.90
20	A	935	U	N3-C2-O2	-7.78	116.75	122.20
1	a	769	C	C6-N1-C1'	-7.78	111.47	120.80
20	A	422	A	N1-C2-N3	7.74	133.17	129.30
20	A	649	C	C5-C6-N1	7.71	124.86	121.00
20	A	644	U	N1-C2-O2	7.71	128.20	122.80
1	a	1446	C	C2-N1-C1'	7.69	127.26	118.80
20	A	602	C	C6-N1-C2	-7.69	117.22	120.30
20	A	935	U	N1-C2-O2	7.68	128.18	122.80
20	A	1213	U	N1-C2-O2	7.68	128.18	122.80
20	A	655	G	C8-N9-C4	7.66	109.46	106.40
1	a	995	C	C6-N1-C1'	-7.65	111.62	120.80
1	a	1125	C	N1-C2-O2	7.63	123.48	118.90
20	A	939	C	N1-C2-O2	7.58	123.45	118.90
1	a	1446	C	N3-C2-O2	-7.58	116.60	121.90
1	a	1152	U	N3-C2-O2	-7.57	116.90	122.20
20	A	2162	G	C4-N9-C1'	-7.56	116.67	126.50
20	A	2506	U	N1-C2-O2	7.55	128.08	122.80
1	a	659	U	N3-C2-O2	-7.54	116.92	122.20
20	A	621	C	C5-C6-N1	7.54	124.77	121.00
20	A	1591	A	C2-N3-C4	7.54	114.37	110.60
1	a	1513	G	N3-C4-N9	-7.53	121.48	126.00
20	A	2082	U	N1-C2-O2	7.50	128.05	122.80
20	A	1882	C	C2-N1-C1'	7.46	127.01	118.80
1	a	1363	U	C5-C6-N1	7.46	126.43	122.70
1	a	1465	U	N3-C2-O2	-7.43	117.00	122.20
20	A	1804	C	C5-C6-N1	7.42	124.71	121.00
20	A	164	U	N1-C2-N3	7.42	119.35	114.90
1	a	634	U	N3-C2-O2	-7.40	117.02	122.20
20	A	607	G	N3-C4-N9	7.39	130.44	126.00
20	A	2826	C	N1-C2-O2	7.38	123.33	118.90
1	a	1482	C	N1-C2-O2	7.37	123.32	118.90
20	A	716	A	N7-C8-N9	7.32	117.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	2417	C	N1-C2-O2	7.32	123.29	118.90
20	A	1448	U	N3-C2-O2	-7.31	117.09	122.20
1	a	1082	C	C5-C6-N1	7.30	124.65	121.00
20	A	709	G	N3-C4-N9	7.29	130.37	126.00
1	a	141	C	N3-C2-O2	-7.29	116.80	121.90
20	A	1584	G	P-O3'-C3'	7.29	128.44	119.70
20	A	1492	G	N3-C4-N9	-7.27	121.64	126.00
20	A	901	U	N3-C2-O2	-7.26	117.11	122.20
20	A	433	U	N3-C2-O2	-7.25	117.12	122.20
21	B	89	C	N3-C2-O2	-7.25	116.83	121.90
20	A	2766	C	N1-C2-O2	7.24	123.24	118.90
20	A	67	C	N1-C2-O2	7.24	123.24	118.90
1	a	1363	U	C2-N1-C1'	7.23	126.38	117.70
1	a	613	U	N3-C2-O2	-7.22	117.15	122.20
20	A	1350	C	C6-N1-C2	-7.21	117.42	120.30
20	A	917	C	N1-C2-O2	7.19	123.22	118.90
20	A	2595	G	C4-N9-C1'	7.19	135.84	126.50
1	a	952	C	N1-C2-O2	7.18	123.21	118.90
21	B	68	C	C6-N1-C1'	-7.15	112.22	120.80
20	A	1146	A	C2-N3-C4	7.15	114.17	110.60
1	a	1091	U	N3-C2-O2	-7.14	117.20	122.20
20	A	1765	C	C6-N1-C2	-7.14	117.45	120.30
20	A	1102	G	N3-C4-N9	7.13	130.28	126.00
1	a	633	C	N1-C2-O2	7.12	123.17	118.90
1	a	862	C	N1-C2-O2	7.12	123.17	118.90
20	A	1130	U	C6-N1-C2	-7.11	116.73	121.00
20	A	1878	U	C2-N1-C1'	7.11	126.24	117.70
21	B	68	C	N3-C2-O2	-7.11	116.92	121.90
1	a	769	C	N1-C2-O2	7.11	123.17	118.90
20	A	1878	U	N1-C2-O2	7.11	127.78	122.80
20	A	607	G	C8-N9-C1'	-7.08	117.79	127.00
1	a	626	C	N1-C2-O2	7.07	123.14	118.90
20	A	1689	A	C2-N3-C4	7.05	114.12	110.60
20	A	2157	C	C6-N1-C2	-7.05	117.48	120.30
20	A	602	C	C2-N1-C1'	7.03	126.53	118.80
20	A	2143	C	N3-C2-O2	-7.03	116.98	121.90
1	a	243	A	C2-N3-C4	-6.98	107.11	110.60
1	a	878	C	C6-N1-C2	-6.98	117.51	120.30
20	A	2048	U	C6-N1-C1'	-6.97	111.44	121.20
1	a	1335	C	C6-N1-C1'	-6.96	112.45	120.80
1	a	534	C	N1-C2-O2	6.96	123.07	118.90
1	a	1061	C	C2-N1-C1'	6.95	126.45	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1193	C	C2-N1-C1'	6.93	126.42	118.80
20	A	2162	G	C8-N9-C1'	6.92	136.00	127.00
20	A	2408	C	N1-C2-O2	6.91	123.05	118.90
20	A	1360	G	N9-C4-C5	6.89	108.16	105.40
1	a	1082	C	N3-C2-O2	-6.89	117.08	121.90
20	A	1434	C	C2-N1-C1'	6.89	126.38	118.80
20	A	709	G	C4-N9-C1'	6.88	135.44	126.50
20	A	2262	C	N1-C2-O2	6.88	123.03	118.90
20	A	602	C	N3-C2-O2	-6.87	117.09	121.90
20	A	1130	U	C5-C6-N1	6.86	126.13	122.70
20	A	2048	U	N1-C2-O2	6.85	127.59	122.80
20	A	901	U	N1-C2-O2	6.84	127.59	122.80
20	A	602	C	N1-C2-O2	6.84	123.00	118.90
20	A	2127	C	N1-C2-O2	6.84	123.00	118.90
20	A	1604	A	P-O3'-C3'	6.83	127.89	119.70
1	a	946	C	N1-C2-O2	6.83	123.00	118.90
20	A	495	C	C2-N1-C1'	6.82	126.31	118.80
1	a	579	U	C2-N1-C1'	6.81	125.87	117.70
20	A	621	C	C6-N1-C2	-6.81	117.58	120.30
20	A	716	A	C8-N9-C4	-6.80	103.08	105.80
20	A	1433	U	N3-C2-O2	-6.80	117.44	122.20
1	a	1306	C	C5-C6-N1	6.80	124.40	121.00
20	A	1883	U	N1-C2-O2	6.80	127.56	122.80
20	A	1511	C	N3-C2-O2	-6.79	117.14	121.90
20	A	2595	G	N3-C4-C5	-6.79	125.21	128.60
1	a	73	C	C5-C6-N1	6.78	124.39	121.00
20	A	164	U	C2-N3-C4	-6.78	122.93	127.00
20	A	1453	U	N1-C2-O2	6.78	127.54	122.80
20	A	1271	U	C2-N1-C1'	6.78	125.83	117.70
20	A	892	U	N3-C2-O2	-6.77	117.46	122.20
20	A	2175	C	C2-N1-C1'	6.77	126.24	118.80
1	a	115	C	N3-C2-O2	-6.76	117.17	121.90
20	A	1393	C	N3-C2-O2	-6.76	117.17	121.90
1	a	1082	C	C6-N1-C2	-6.73	117.61	120.30
20	A	2048	U	N3-C2-O2	-6.72	117.49	122.20
20	A	2480	C	C6-N1-C2	-6.72	117.61	120.30
20	A	1695	C	C6-N1-C2	-6.71	117.62	120.30
20	A	2697	C	N1-C2-O2	6.70	122.92	118.90
20	A	2597	G	C4-N9-C1'	-6.70	117.79	126.50
20	A	709	G	C8-N9-C1'	-6.69	118.30	127.00
1	a	1306	C	C6-N1-C1'	-6.68	112.78	120.80
1	a	221	C	C5-C6-N1	6.66	124.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1453	U	C6-N1-C1'	-6.66	111.88	121.20
1	a	952	C	C2-N1-C1'	6.63	126.09	118.80
1	a	995	C	C5-C6-N1	6.61	124.31	121.00
20	A	2208	C	C2-N1-C1'	6.61	126.07	118.80
20	A	2262	C	N3-C2-O2	-6.61	117.27	121.90
20	A	1882	C	N1-C2-O2	6.60	122.86	118.90
1	a	826	C	N1-C2-O2	6.60	122.86	118.90
20	A	164	U	N3-C2-O2	-6.59	117.58	122.20
20	A	939	C	N3-C2-O2	-6.59	117.29	121.90
20	A	1128	A	N3-C4-N9	6.59	132.67	127.40
20	A	527	C	N1-C2-O2	6.59	122.85	118.90
20	A	2819	U	N1-C2-O2	6.58	127.40	122.80
1	a	1513	G	C8-N9-C1'	6.57	135.54	127.00
20	A	2630	C	C2-N1-C1'	6.57	126.02	118.80
1	a	1173	C	C2-N1-C1'	6.56	126.02	118.80
1	a	1040	U	C2-N1-C1'	6.55	125.56	117.70
20	A	2570	C	N1-C2-O2	6.54	122.83	118.90
1	a	178	A	C8-N9-C4	-6.54	103.18	105.80
20	A	1047	C	C2-N1-C1'	6.54	125.99	118.80
20	A	1790	G	N3-C4-N9	6.54	129.92	126.00
20	A	1827	U	N3-C2-O2	-6.54	117.62	122.20
20	A	2480	C	C5-C6-N1	6.54	124.27	121.00
20	A	312	U	P-O3'-C3'	6.51	127.52	119.70
20	A	2162	G	O4'-C1'-N9	6.51	113.41	108.20
1	a	115	C	N1-C2-O2	6.51	122.80	118.90
1	a	1465	U	C2-N1-C1'	6.51	125.51	117.70
20	A	2417	C	C2-N1-C1'	6.50	125.95	118.80
1	a	867	C	C6-N1-C2	-6.49	117.70	120.30
20	A	607	G	N3-C4-C5	-6.49	125.36	128.60
20	A	2595	G	N3-C4-N9	6.49	129.89	126.00
20	A	2826	C	C6-N1-C1'	-6.49	113.01	120.80
1	a	826	C	C2-N1-C1'	6.48	125.92	118.80
20	A	1104	C	N3-C2-O2	-6.46	117.38	121.90
20	A	1197	G	N3-C4-N9	6.46	129.88	126.00
1	a	952	C	N3-C2-O2	-6.43	117.39	121.90
20	A	1360	G	C5-C6-O6	6.43	132.46	128.60
1	a	635	C	N1-C2-O2	6.43	122.76	118.90
20	A	2488	C	N3-C2-O2	-6.42	117.40	121.90
20	A	1148	U	C2-N1-C1'	6.40	125.38	117.70
20	A	730	C	N3-C2-O2	-6.40	117.42	121.90
20	A	4	U	N1-C2-O2	6.40	127.28	122.80
20	A	649	C	C4-C5-C6	-6.39	114.21	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1306	C	C6-N1-C2	-6.34	117.76	120.30
20	A	2488	C	C2-N1-C1'	6.34	125.78	118.80
20	A	1551	U	C5-C6-N1	6.34	125.87	122.70
1	a	73	C	C6-N1-C2	-6.33	117.77	120.30
1	a	1363	U	N1-C2-O2	6.33	127.23	122.80
20	A	1689	A	N3-C4-C5	-6.33	122.37	126.80
20	A	1271	U	N3-C2-O2	-6.32	117.78	122.20
20	A	2157	C	C5-C6-N1	6.32	124.16	121.00
20	A	2597	G	N3-C4-N9	-6.32	122.21	126.00
20	A	137	U	N1-C2-O2	6.32	127.22	122.80
1	a	633	C	N3-C2-O2	-6.31	117.48	121.90
20	A	4	U	C2-N1-C1'	6.31	125.27	117.70
1	a	613	U	N1-C2-O2	6.30	127.21	122.80
20	A	1588	C	N1-C2-O2	6.30	122.68	118.90
1	a	1025	U	N1-C2-O2	6.29	127.20	122.80
20	A	2044	A	O4'-C1'-N9	6.27	113.22	108.20
21	B	92	U	N1-C2-O2	6.27	127.19	122.80
1	a	867	C	N1-C2-O2	6.27	122.66	118.90
20	A	1878	U	N3-C2-O2	-6.26	117.82	122.20
20	A	992	G	N3-C4-N9	6.26	129.75	126.00
20	A	1934	C	C6-N1-C2	-6.26	117.80	120.30
20	A	2082	U	N3-C2-O2	-6.26	117.82	122.20
1	a	1513	G	C4-N9-C1'	-6.25	118.37	126.50
20	A	2127	C	C2-N1-C1'	6.25	125.67	118.80
20	A	1448	U	C2-N1-C1'	6.24	125.19	117.70
20	A	2214	C	N1-C2-O2	6.24	122.64	118.90
1	a	1009	G	N3-C4-N9	6.24	129.74	126.00
20	A	137	U	N3-C2-O2	-6.24	117.83	122.20
20	A	2766	C	C2-N1-C1'	6.23	125.66	118.80
20	A	1434	C	N1-C2-O2	6.23	122.64	118.90
20	A	1492	G	N3-C4-C5	6.23	131.72	128.60
20	A	1047	C	C6-N1-C2	-6.23	117.81	120.30
20	A	2891	C	N3-C2-O2	-6.22	117.54	121.90
1	a	498	C	C2-N1-C1'	6.22	125.64	118.80
11	l	39	ASN	C-N-CA	6.22	137.25	121.70
20	A	2418	C	N3-C2-O2	-6.22	117.55	121.90
20	A	1115	C	C6-N1-C2	-6.22	117.81	120.30
1	a	243	A	N3-C4-N9	-6.21	122.43	127.40
20	A	901	U	C2-N1-C1'	6.21	125.15	117.70
38	V	71	ILE	C-N-CA	6.20	137.21	121.70
20	A	1508	G	C8-N9-C4	-6.20	103.92	106.40
20	A	1130	U	C6-N1-C1'	-6.20	112.52	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	383	U	C2-N1-C1'	6.20	125.13	117.70
21	B	92	U	N3-C2-O2	-6.19	117.86	122.20
1	a	331	C	C6-N1-C2	-6.18	117.83	120.30
1	a	1455	U	N1-C2-O2	6.18	127.13	122.80
1	a	920	U	N3-C2-O2	-6.17	117.88	122.20
20	A	2696	G	N3-C4-N9	6.17	129.70	126.00
20	A	475	C	N1-C2-O2	6.17	122.60	118.90
20	A	2277	C	C6-N1-C2	-6.17	117.83	120.30
1	a	862	C	C2-N1-C1'	6.16	125.57	118.80
1	a	1162	C	N1-C2-O2	6.16	122.59	118.90
20	A	422	A	C8-N9-C4	-6.15	103.34	105.80
20	A	1350	C	C2-N1-C1'	6.15	125.56	118.80
1	a	1082	C	C6-N1-C1'	-6.14	113.44	120.80
1	a	579	U	N1-C2-O2	6.13	127.09	122.80
20	A	1689	A	N3-C4-N9	6.13	132.30	127.40
20	A	1802	C	N1-C2-O2	6.13	122.58	118.90
20	A	1434	C	C5-C6-N1	6.13	124.06	121.00
20	A	1360	G	N1-C6-O6	-6.12	116.23	119.90
1	a	1173	C	C6-N1-C2	-6.12	117.85	120.30
20	A	4	U	N3-C2-O2	-6.12	117.92	122.20
20	A	956	C	N1-C2-O2	6.11	122.57	118.90
20	A	1591	A	C4-N9-C1'	6.11	137.30	126.30
20	A	931	C	C2-N1-C1'	6.11	125.52	118.80
20	A	1039	U	N3-C2-O2	-6.10	117.93	122.20
20	A	980	G	N1-C6-O6	-6.08	116.25	119.90
20	A	1622	U	N3-C2-O2	-6.08	117.94	122.20
20	A	2597	G	C8-N9-C1'	6.08	134.91	127.00
1	a	952	C	C5-C6-N1	6.08	124.04	121.00
20	A	2696	G	N3-C4-C5	-6.07	125.56	128.60
20	A	1130	U	O4'-C1'-N1	6.06	113.05	108.20
1	a	946	C	C6-N1-C1'	-6.05	113.54	120.80
20	A	913	U	C2-N1-C1'	6.05	124.96	117.70
20	A	2595	G	C8-N9-C1'	-6.05	119.13	127.00
20	A	1366	C	N1-C2-O2	6.05	122.53	118.90
20	A	77	C	C5-C6-N1	6.04	124.02	121.00
1	a	108	U	N3-C2-O2	-6.04	117.97	122.20
20	A	1216	G	N7-C8-N9	6.04	116.12	113.10
1	a	634	U	C6-N1-C1'	-6.04	112.74	121.20
20	A	2311	C	C6-N1-C2	-6.03	117.89	120.30
20	A	2819	U	N3-C2-O2	-6.03	117.98	122.20
20	A	1148	U	N3-C2-O2	-6.02	117.98	122.20
20	A	657	C	C2-N1-C1'	6.02	125.42	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1115	C	N1-C2-O2	6.01	122.51	118.90
1	a	649	C	N3-C2-O2	-6.01	117.69	121.90
20	A	2520	U	C2-N1-C1'	6.01	124.91	117.70
20	A	550	U	C2-N1-C1'	6.01	124.91	117.70
1	a	626	C	N3-C2-O2	-6.01	117.69	121.90
20	A	424	A	C2-N3-C4	6.00	113.60	110.60
20	A	2042	U	N3-C2-O2	-6.00	118.00	122.20
1	a	1455	U	N3-C2-O2	-6.00	118.00	122.20
1	a	284	C	C2-N1-C1'	6.00	125.39	118.80
20	A	1431	A	O4'-C1'-N9	5.99	112.99	108.20
1	a	560	C	N1-C2-O2	5.99	122.49	118.90
1	a	1061	C	N1-C2-O2	5.98	122.49	118.90
1	a	141	C	C2-N1-C1'	5.98	125.38	118.80
20	A	2175	C	C5-C6-N1	5.97	123.99	121.00
20	A	2010	C	N3-C2-O2	-5.96	117.72	121.90
1	a	658	C	C6-N1-C2	-5.96	117.92	120.30
20	A	1797	A	C8-N9-C4	-5.96	103.42	105.80
20	A	2697	C	N3-C2-O2	-5.96	117.73	121.90
20	A	963	C	C5-C6-N1	5.94	123.97	121.00
20	A	1193	C	C5-C6-N1	5.94	123.97	121.00
1	a	1087	C	C6-N1-C2	-5.94	117.93	120.30
1	a	1217	U	N1-C2-O2	5.94	126.96	122.80
21	B	96	G	C4-N9-C1'	5.93	134.22	126.50
1	a	769	C	N3-C2-O2	-5.93	117.75	121.90
20	A	2163	U	C5-C6-N1	5.93	125.67	122.70
20	A	2661	U	N1-C2-O2	5.93	126.95	122.80
1	a	560	C	C2-N1-C1'	5.93	125.32	118.80
1	a	1105	G	C5-C6-O6	5.92	132.15	128.60
1	a	235	G	N3-C4-N9	5.91	129.55	126.00
1	a	579	U	N3-C2-O2	-5.91	118.07	122.20
20	A	605	U	N3-C2-O2	-5.90	118.07	122.20
20	A	2317	G	P-O3'-C3'	5.90	126.78	119.70
20	A	2417	C	N3-C2-O2	-5.90	117.77	121.90
20	A	1092	C	C6-N1-C1'	-5.89	113.73	120.80
20	A	580	U	N3-C2-O2	-5.89	118.08	122.20
20	A	1148	U	N1-C2-O2	5.89	126.92	122.80
20	A	1790	G	C4-N9-C1'	5.89	134.16	126.50
20	A	2570	C	C6-N1-C2	-5.89	117.94	120.30
1	a	243	A	N3-C4-C5	5.88	130.92	126.80
1	a	64	C	C6-N1-C2	-5.88	117.95	120.30
20	A	2327	C	N1-C2-O2	5.88	122.42	118.90
20	A	605	U	N1-C2-O2	5.86	126.90	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	759	C	N1-C2-O2	5.86	122.41	118.90
20	A	1472	C	C6-N1-C2	-5.85	117.96	120.30
20	A	642	G	N1-C6-O6	-5.84	116.39	119.90
20	A	1271	U	N1-C2-O2	5.83	126.88	122.80
20	A	2794	G	C4-N9-C1'	5.83	134.08	126.50
20	A	2570	C	N3-C2-O2	-5.83	117.82	121.90
20	A	2885	C	N1-C2-O2	5.83	122.40	118.90
20	A	2143	C	N1-C2-O2	5.82	122.39	118.90
20	A	1102	G	N3-C4-C5	-5.82	125.69	128.60
20	A	1758	C	N3-C2-O2	-5.82	117.83	121.90
20	A	2078	C	C6-N1-C2	-5.82	117.97	120.30
20	A	422	A	N3-C4-N9	-5.81	122.75	127.40
20	A	1883	U	N3-C2-O2	-5.81	118.13	122.20
1	a	1087	C	C5-C6-N1	5.80	123.90	121.00
20	A	325	U	N1-C2-O2	5.80	126.86	122.80
1	a	305	C	C6-N1-C2	-5.80	117.98	120.30
1	a	401	C	N1-C2-O2	5.79	122.38	118.90
20	A	454	C	N1-C2-O2	5.78	122.37	118.90
20	A	1127	G	N3-C2-N2	-5.78	115.86	119.90
20	A	1695	C	C2-N1-C1'	5.77	125.14	118.80
1	a	159	C	N1-C2-O2	5.76	122.36	118.90
20	A	1844	C	N1-C2-O2	5.76	122.36	118.90
20	A	1530	A	P-O3'-C3'	5.76	126.61	119.70
20	A	1109	A	O4'-C1'-N9	5.76	112.81	108.20
20	A	2193	C	C6-N1-C2	-5.76	118.00	120.30
1	a	73	C	C2-N1-C1'	5.75	125.12	118.80
20	A	527	C	N3-C2-O2	-5.74	117.88	121.90
20	A	2596	G	N1-C6-O6	-5.72	116.47	119.90
1	a	427	A	P-O3'-C3'	5.72	126.57	119.70
20	A	607	G	C6-C5-N7	-5.72	126.97	130.40
20	A	1718	C	C6-N1-C2	-5.71	118.01	120.30
1	a	860	C	C5-C6-N1	5.71	123.86	121.00
20	A	1156	C	N1-C2-O2	5.71	122.33	118.90
20	A	2717	C	N1-C2-O2	5.71	122.33	118.90
20	A	1472	C	C5-C6-N1	5.71	123.85	121.00
1	a	1373	U	C5-C6-N1	5.71	125.55	122.70
20	A	1569	G	C5-C6-O6	5.70	132.02	128.60
1	a	1009	G	C4-N9-C1'	5.70	133.91	126.50
20	A	2054	U	N3-C2-O2	-5.70	118.21	122.20
20	A	709	G	N3-C4-C5	-5.70	125.75	128.60
20	A	2311	C	C5-C6-N1	5.70	123.85	121.00
20	A	2116	U	N3-C2-O2	-5.69	118.22	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	963	C	C6-N1-C2	-5.69	118.02	120.30
20	A	1605	C	P-O3'-C3'	5.69	126.53	119.70
1	a	34	U	N3-C2-O2	-5.69	118.22	122.20
1	a	1517	C	C2-N1-C1'	5.68	125.05	118.80
20	A	2055	U	C5-C6-N1	5.68	125.54	122.70
1	a	766	U	N3-C2-O2	-5.67	118.23	122.20
1	a	1019	G	C8-N9-C4	-5.67	104.13	106.40
1	a	812	C	N3-C2-O2	-5.67	117.93	121.90
1	a	867	C	N3-C2-O2	-5.67	117.93	121.90
20	A	2054	U	N1-C2-O2	5.67	126.77	122.80
20	A	917	C	N3-C2-O2	-5.67	117.93	121.90
1	a	141	C	C6-N1-C2	-5.67	118.03	120.30
1	a	1513	G	N9-C4-C5	5.66	107.66	105.40
1	a	1025	U	N3-C2-O2	-5.66	118.24	122.20
1	a	1196	G	N3-C4-N9	-5.66	122.61	126.00
1	a	141	C	C5-C6-N1	5.65	123.83	121.00
1	a	159	C	N3-C2-O2	-5.65	117.94	121.90
20	A	2082	U	C6-N1-C1'	-5.65	113.29	121.20
20	A	235	G	C4-N9-C1'	5.65	133.84	126.50
1	a	73	C	N3-C2-O2	-5.64	117.95	121.90
20	A	1548	C	C2-N1-C1'	5.63	125.00	118.80
1	a	122	G	N3-C4-N9	5.63	129.38	126.00
20	A	1804	C	C2-N1-C1'	5.62	124.99	118.80
20	A	2327	C	C2-N1-C1'	5.62	124.99	118.80
20	A	574	C	C5-C6-N1	5.62	123.81	121.00
20	A	114	U	C2-N1-C1'	5.61	124.44	117.70
1	a	443	G	C5-C6-O6	-5.61	125.23	128.60
1	a	1091	U	N1-C2-O2	5.61	126.72	122.80
20	A	1025	C	C6-N1-C2	-5.61	118.06	120.30
20	A	1680	C	N1-C2-O2	5.61	122.26	118.90
20	A	938	C	C5-C6-N1	5.61	123.80	121.00
20	A	1359	G	C5-C6-N1	5.61	114.30	111.50
20	A	2753	U	N1-C2-O2	5.60	126.72	122.80
20	A	1213	U	C2-N1-C1'	5.60	124.42	117.70
20	A	1585	U	N1-C2-O2	5.59	126.72	122.80
20	A	1561	U	N1-C2-O2	5.59	126.71	122.80
20	A	1367	C	N1-C2-O2	5.58	122.25	118.90
20	A	2408	C	N3-C2-O2	-5.58	117.99	121.90
20	A	1755	C	C6-N1-C2	-5.57	118.07	120.30
20	A	1885	C	C6-N1-C2	-5.57	118.07	120.30
20	A	1039	U	C2-N1-C1'	5.56	124.38	117.70
20	A	1327	U	N3-C2-O2	-5.56	118.31	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	2162	G	C6-C5-N7	5.56	133.74	130.40
20	A	1102	G	C6-C5-N7	-5.55	127.07	130.40
20	A	1907	C	N1-C2-O2	5.55	122.23	118.90
1	a	348	C	N1-C2-O2	5.55	122.23	118.90
1	a	1044	C	C6-N1-C2	-5.55	118.08	120.30
1	a	1428	A	N7-C8-N9	5.54	116.57	113.80
20	A	69	C	N1-C2-O2	5.54	122.22	118.90
1	a	659	U	N1-C2-O2	5.53	126.67	122.80
20	A	2520	U	N1-C2-O2	5.53	126.67	122.80
20	A	649	C	N1-C2-O2	5.53	122.22	118.90
1	a	373	U	N3-C2-O2	-5.53	118.33	122.20
20	A	1622	U	N1-C2-O2	5.53	126.67	122.80
1	a	305	C	C5-C6-N1	5.52	123.76	121.00
20	A	1293	G	C4-N9-C1'	5.52	133.68	126.50
20	A	1349	U	C6-N1-C1'	-5.51	113.48	121.20
20	A	2850	G	C4-N9-C1'	5.51	133.66	126.50
20	A	638	C	C2-N1-C1'	5.51	124.86	118.80
1	a	812	C	N1-C2-O2	5.51	122.20	118.90
20	A	1925	U	C5-C6-N1	5.51	125.45	122.70
20	A	2766	C	N3-C2-O2	-5.51	118.05	121.90
20	A	325	U	N3-C2-O2	-5.50	118.35	122.20
1	a	1061	C	C6-N1-C1'	-5.49	114.21	120.80
21	B	114	C	C6-N1-C2	-5.49	118.10	120.30
20	A	1128	A	N7-C8-N9	5.49	116.54	113.80
20	A	1638	C	N1-C2-O2	5.49	122.19	118.90
21	B	114	C	C5-C6-N1	5.49	123.74	121.00
1	a	551	C	O5'-P-OP2	-5.49	100.76	105.70
20	A	1638	C	C2-N1-C1'	5.49	124.83	118.80
20	A	1850	C	C6-N1-C2	-5.49	118.11	120.30
20	A	2506	U	C2-N1-C1'	5.48	124.28	117.70
20	A	1501	A	N3-C4-N9	5.48	131.78	127.40
20	A	156	U	C5-C6-N1	5.48	125.44	122.70
20	A	1304	U	C2-N1-C1'	5.47	124.27	117.70
20	A	1436	U	N3-C4-O4	5.47	123.23	119.40
20	A	1103	G	N3-C2-N2	-5.47	116.07	119.90
1	a	1217	U	C2-N1-C1'	5.47	124.26	117.70
1	a	1125	C	N3-C2-O2	-5.46	118.08	121.90
20	A	1585	U	N3-C2-O2	-5.46	118.38	122.20
20	A	1758	C	C6-N1-C1'	-5.46	114.25	120.80
20	A	1882	C	C5-C6-N1	5.46	123.73	121.00
1	a	867	C	C2-N1-C1'	5.45	124.79	118.80
20	A	1128	A	C6-C5-N7	-5.45	128.49	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1449	U	C5-C6-N1	5.45	125.42	122.70
20	A	1802	C	C2-N1-C1'	5.45	124.80	118.80
20	A	1501	A	C2-N3-C4	5.45	113.33	110.60
20	A	941	A	C4-N9-C1'	5.44	136.10	126.30
20	A	956	C	C6-N1-C2	-5.44	118.12	120.30
1	a	1301	U	N1-C2-O2	5.44	126.61	122.80
20	A	2307	C	C5-C6-N1	5.44	123.72	121.00
20	A	1883	U	C5-C6-N1	5.43	125.42	122.70
20	A	920	G	C4-N9-C1'	-5.43	119.44	126.50
20	A	2208	C	N1-C2-O2	5.43	122.16	118.90
20	A	1844	C	N3-C2-O2	-5.42	118.10	121.90
20	A	1140	C	C6-N1-C2	-5.42	118.13	120.30
1	a	214	U	N1-C2-O2	5.42	126.59	122.80
20	A	1453	U	N3-C2-O2	-5.42	118.41	122.20
20	A	1492	G	C8-N9-C1'	5.42	134.04	127.00
20	A	67	C	C2-N1-C1'	5.41	124.75	118.80
1	a	534	C	N3-C2-O2	-5.41	118.11	121.90
20	A	2116	U	N1-C2-O2	5.41	126.59	122.80
20	A	1631	A	N3-C4-N9	5.41	131.72	127.40
20	A	1882	C	C6-N1-C2	-5.40	118.14	120.30
21	B	58	C	C5-C6-N1	5.40	123.70	121.00
1	a	1512	C	C6-N1-C2	-5.39	118.14	120.30
20	A	2078	C	C2-N1-C1'	5.39	124.73	118.80
1	a	1306	C	N3-C2-O2	-5.39	118.13	121.90
1	a	1427	C	C6-N1-C2	-5.39	118.14	120.30
20	A	549	C	C6-N1-C2	-5.39	118.15	120.30
20	A	1790	G	C8-N9-C1'	-5.38	120.00	127.00
20	A	892	U	N1-C2-O2	5.38	126.56	122.80
1	a	248	C	C6-N1-C2	-5.37	118.15	120.30
20	A	423	C	C6-N1-C2	-5.37	118.15	120.30
20	A	1108	G	C4-N9-C1'	5.37	133.48	126.50
20	A	1695	C	N1-C2-O2	5.37	122.12	118.90
20	A	657	C	C6-N1-C2	-5.37	118.15	120.30
20	A	1541	C	N3-C2-O2	-5.37	118.14	121.90
1	a	108	U	N1-C2-O2	5.37	126.56	122.80
20	A	102	G	C2-N3-C4	-5.37	109.22	111.90
20	A	906	C	C2-N1-C1'	5.36	124.70	118.80
1	a	635	C	N3-C2-O2	-5.36	118.15	121.90
20	A	1883	U	C2-N1-C1'	5.36	124.13	117.70
20	A	1703	C	C6-N1-C2	-5.36	118.16	120.30
20	A	956	C	N3-C2-O2	-5.35	118.15	121.90
1	a	909	C	N1-C2-O2	5.35	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	2455	C	N1-C2-O2	5.35	122.11	118.90
20	A	2474	U	N1-C2-O2	5.35	126.54	122.80
20	A	1427	U	N3-C2-O2	-5.35	118.46	122.20
21	B	35	C	N1-C2-O2	5.35	122.11	118.90
20	A	772	C	C2-N1-C1'	5.34	124.68	118.80
1	a	625	G	C4-N9-C1'	5.34	133.45	126.50
20	A	906	C	N1-C2-O2	5.34	122.11	118.90
1	a	1159	G	N1-C6-O6	-5.34	116.69	119.90
1	a	1373	U	C2-N1-C1'	5.34	124.11	117.70
20	A	1790	G	C6-C5-N7	-5.34	127.19	130.40
20	A	2082	U	C5-C6-N1	5.34	125.37	122.70
1	a	214	U	N3-C2-O2	-5.34	118.47	122.20
20	A	67	C	N3-C2-O2	-5.34	118.16	121.90
20	A	2143	C	C6-N1-C2	-5.34	118.17	120.30
1	a	1057	G	N3-C4-N9	-5.33	122.80	126.00
20	A	837	U	C2-N1-C1'	5.33	124.10	117.70
20	A	475	C	N3-C2-O2	-5.33	118.17	121.90
1	a	635	C	C2-N1-C1'	5.33	124.66	118.80
20	A	2826	C	N3-C2-O2	-5.33	118.17	121.90
20	A	2163	U	C2-N1-C1'	5.32	124.09	117.70
20	A	571	A	C4-N9-C1'	5.32	135.88	126.30
20	A	1039	U	N1-C2-O2	5.32	126.53	122.80
20	A	63	C	O4'-C1'-N1	5.32	112.45	108.20
20	A	1648	C	C6-N1-C2	-5.32	118.17	120.30
20	A	2858	U	N3-C2-O2	-5.32	118.48	122.20
20	A	555	C	C6-N1-C2	-5.32	118.17	120.30
31	O	41	ARG	CA-CB-CG	5.31	125.09	113.40
31	O	41	ARG	CB-CG-CD	-5.31	97.78	111.60
20	A	1449	U	C2-N1-C1'	5.31	124.07	117.70
1	a	1440	A	O4'-C1'-N9	5.31	112.45	108.20
20	A	1569	G	C8-N9-C4	-5.31	104.28	106.40
20	A	2127	C	N3-C2-O2	-5.31	118.19	121.90
20	A	237	U	N3-C2-O2	-5.31	118.49	122.20
20	A	1271	U	P-O3'-C3'	5.30	126.06	119.70
20	A	2734	U	N3-C2-O2	-5.29	118.49	122.20
1	a	1217	U	P-O3'-C3'	5.29	126.05	119.70
1	a	884	C	N1-C2-O2	5.29	122.07	118.90
20	A	2311	C	C2-N1-C1'	5.29	124.62	118.80
1	a	1446	C	C6-N1-C1'	-5.29	114.46	120.80
1	a	401	C	N3-C2-O2	-5.29	118.20	121.90
1	a	946	C	C5-C6-N1	5.29	123.64	121.00
20	A	1631	A	C4-N9-C1'	5.28	135.80	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	71	U	N3-C2-O2	-5.28	118.51	122.20
1	a	331	C	C2-N1-C1'	5.28	124.60	118.80
1	a	939	A	N7-C8-N9	5.27	116.44	113.80
20	A	2568	U	C2-N1-C1'	-5.27	111.37	117.70
20	A	1436	U	C5-C4-O4	-5.27	122.74	125.90
20	A	2455	C	C2-N1-C1'	5.27	124.60	118.80
20	A	2408	C	C2-N1-C1'	5.27	124.60	118.80
20	A	1695	C	C5-C6-N1	5.26	123.63	121.00
21	B	89	C	N1-C2-O2	5.26	122.06	118.90
20	A	693	U	P-O3'-C3'	5.26	126.01	119.70
1	a	601	C	C6-N1-C2	-5.26	118.20	120.30
1	a	1446	C	C6-N1-C2	-5.26	118.20	120.30
20	A	2175	C	C6-N1-C2	-5.25	118.20	120.30
20	A	1689	A	C4-N9-C1'	5.25	135.75	126.30
38	V	60	GLU	C-N-CA	5.25	134.83	121.70
1	a	278	A	O4'-C1'-N9	5.25	112.40	108.20
20	A	2417	C	C6-N1-C2	-5.25	118.20	120.30
20	A	1408	U	N1-C2-O2	5.24	126.47	122.80
20	A	550	U	N1-C2-O2	5.24	126.47	122.80
1	a	457	U	N3-C2-O2	-5.24	118.53	122.20
20	A	742	U	N3-C2-O2	-5.24	118.53	122.20
1	a	1040	U	N1-C2-O2	5.24	126.47	122.80
1	a	6	G	O4'-C1'-N9	5.24	112.39	108.20
20	A	1532	A	N1-C6-N6	5.23	121.74	118.60
20	A	2576	U	N3-C2-O2	-5.23	118.54	122.20
20	A	1548	C	C6-N1-C2	-5.22	118.21	120.30
1	a	107	G	N3-C2-N2	-5.22	116.25	119.90
1	a	1363	U	N3-C2-O2	-5.22	118.55	122.20
20	A	1193	C	N1-C2-O2	5.22	122.03	118.90
20	A	2630	C	C5-C6-N1	5.21	123.61	121.00
1	a	451	C	C2-N1-C1'	5.21	124.53	118.80
2	c	195	LEU	CA-CB-CG	5.21	127.29	115.30
20	A	535	G	N9-C4-C5	-5.21	103.31	105.40
20	A	2597	G	N3-C4-C5	5.21	131.21	128.60
1	a	1009	G	C8-N9-C1'	-5.21	120.23	127.00
20	A	121	G	C4-C5-N7	5.21	112.88	110.80
1	a	633	C	C2-N1-C1'	5.21	124.53	118.80
20	A	1304	U	N1-C2-O2	5.20	126.44	122.80
20	A	772	C	N1-C2-O2	5.20	122.02	118.90
1	a	1105	G	N3-C4-N9	-5.20	122.88	126.00
21	B	96	G	C8-N9-C1'	-5.20	120.24	127.00
1	a	597	C	N3-C2-O2	-5.20	118.26	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	335	G	N3-C4-N9	5.19	129.12	126.00
20	A	853	U	N3-C2-O2	-5.19	118.57	122.20
1	a	1152	U	C6-N1-C1'	-5.19	113.94	121.20
20	A	1591	A	C8-N9-C4	-5.19	103.72	105.80
20	A	2706	C	N1-C2-O2	5.19	122.01	118.90
20	A	2057	C	C6-N1-C2	-5.18	118.23	120.30
1	a	350	C	C6-N1-C2	-5.18	118.23	120.30
1	a	1183	C	N1-C2-O2	5.18	122.01	118.90
20	A	1434	C	C6-N1-C1'	-5.18	114.59	120.80
1	a	235	G	C4-N9-C1'	5.17	133.23	126.50
20	A	2200	U	C5-C6-N1	5.17	125.29	122.70
1	a	1387	U	N3-C2-O2	-5.17	118.58	122.20
20	A	1366	C	N3-C2-O2	-5.17	118.28	121.90
20	A	2734	U	N1-C2-O2	5.17	126.42	122.80
1	a	1044	C	C5-C6-N1	5.17	123.59	121.00
20	A	2701	U	N3-C2-O2	-5.17	118.58	122.20
20	A	1359	G	N1-C6-O6	-5.17	116.80	119.90
1	a	470	A	O4'-C1'-N9	5.16	112.33	108.20
20	A	1104	C	C2-N1-C1'	5.16	124.47	118.80
20	A	499	U	N3-C2-O2	-5.16	118.59	122.20
20	A	848	G	C5-C6-O6	5.16	131.70	128.60
1	a	1113	C	C6-N1-C2	-5.16	118.24	120.30
20	A	917	C	C2-N1-C1'	5.16	124.47	118.80
20	A	1146	A	N3-C4-C5	-5.16	123.19	126.80
20	A	1360	G	C8-N9-C1'	5.16	133.70	127.00
20	A	1691	C	C6-N1-C2	-5.16	118.24	120.30
20	A	112	U	N3-C2-O2	-5.15	118.59	122.20
20	A	1569	G	N9-C4-C5	5.15	107.46	105.40
20	A	1363	C	N1-C2-O2	5.15	121.99	118.90
20	A	1588	C	N3-C2-O2	-5.15	118.30	121.90
20	A	2307	C	C2-N1-C1'	5.15	124.46	118.80
20	A	887	G	C2-N3-C4	5.15	114.47	111.90
1	a	1022	C	C6-N1-C2	-5.14	118.24	120.30
1	a	1091	U	C2-N1-C1'	5.14	123.87	117.70
20	A	1146	A	N3-C4-N9	5.14	131.51	127.40
20	A	602	C	C5-C6-N1	5.14	123.57	121.00
20	A	759	C	N3-C2-O2	-5.14	118.30	121.90
1	a	1162	C	C5-C6-N1	5.14	123.57	121.00
20	A	935	U	C6-N1-C2	-5.14	117.92	121.00
1	a	579	U	C6-N1-C1'	-5.14	114.01	121.20
20	A	655	G	N9-C4-C5	-5.14	103.34	105.40
20	A	1359	G	O4'-C1'-N9	5.13	112.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	2794	G	N3-C4-N9	5.13	129.08	126.00
1	a	1301	U	N3-C2-O2	-5.13	118.61	122.20
1	a	867	C	C5-C6-N1	5.13	123.56	121.00
20	A	203	U	N1-C2-O2	5.13	126.39	122.80
1	a	649	C	C5-C6-N1	5.13	123.56	121.00
20	A	1197	G	N9-C4-C5	-5.13	103.35	105.40
20	A	1293	G	C8-N9-C1'	-5.13	120.34	127.00
20	A	1359	G	N3-C4-C5	-5.12	126.04	128.60
20	A	1831	G	N3-C4-N9	5.12	129.07	126.00
20	A	1907	C	N3-C2-O2	-5.12	118.31	121.90
1	a	739	G	N3-C4-N9	5.11	129.07	126.00
20	A	716	A	C5-N7-C8	-5.11	101.34	103.90
20	A	1971	C	C2-N1-C1'	5.11	124.42	118.80
1	a	1548	U	N1-C2-O2	5.11	126.38	122.80
1	a	73	C	C2-N3-C4	5.11	122.45	119.90
20	A	102	G	N3-C4-C5	5.11	131.15	128.60
20	A	1095	G	N7-C8-N9	5.11	115.65	113.10
20	A	1317	G	C4-N9-C1'	5.11	133.14	126.50
1	a	498	C	N1-C2-O2	5.10	121.96	118.90
22	C	37	LEU	CB-CG-CD2	-5.10	102.33	111.00
20	A	114	U	N3-C2-O2	-5.10	118.63	122.20
20	A	1128	A	C5-C6-N6	-5.10	119.62	123.70
20	A	140	U	N3-C2-O2	-5.10	118.63	122.20
20	A	1047	C	C5-C6-N1	5.09	123.55	121.00
20	A	1970	U	N1-C2-O2	5.09	126.36	122.80
1	a	250	C	N1-C2-O2	5.09	121.95	118.90
1	a	498	C	C6-N1-C1'	-5.09	114.70	120.80
20	A	495	C	C6-N1-C1'	-5.09	114.70	120.80
1	a	578	A	C4-N9-C1'	5.08	135.45	126.30
20	A	887	G	N3-C4-C5	-5.08	126.06	128.60
20	A	1258	U	N1-C2-O2	5.08	126.36	122.80
20	A	1574	C	N1-C2-O2	5.08	121.94	118.90
1	a	1217	U	N3-C2-O2	-5.07	118.65	122.20
20	A	2794	G	N3-C4-C5	-5.07	126.06	128.60
21	B	109	C	N3-C2-O2	-5.07	118.35	121.90
20	A	1605	C	OP2-P-O3'	5.07	116.35	105.20
1	a	250	C	C2-N1-C1'	5.06	124.37	118.80
20	A	1631	A	C8-N9-C1'	-5.06	118.59	127.70
1	a	487	A	N3-C4-N9	5.06	131.45	127.40
1	a	1311	C	C6-N1-C2	-5.06	118.28	120.30
1	a	1445	C	C2-N1-C1'	5.06	124.36	118.80
20	A	943	U	C2-N1-C1'	5.06	123.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	826	C	C5-C6-N1	5.05	123.53	121.00
20	A	476	C	C6-N1-C2	-5.05	118.28	120.30
1	a	1309	C	C5-C6-N1	5.05	123.52	121.00
20	A	458	C	C2-N1-C1'	5.05	124.35	118.80
20	A	849	G	N1-C6-O6	-5.05	116.87	119.90
20	A	992	G	N3-C4-C5	-5.05	126.08	128.60
1	a	1086	U	N1-C2-O2	5.04	126.33	122.80
1	a	1144	C	C6-N1-C2	-5.04	118.28	120.30
20	A	1433	U	N1-C2-O2	5.04	126.33	122.80
20	A	1623	C	N3-C2-O2	-5.04	118.37	121.90
20	A	730	C	N1-C2-O2	5.04	121.92	118.90
20	A	1803	A	N7-C8-N9	5.04	116.32	113.80
1	a	766	U	N1-C2-O2	5.04	126.33	122.80
20	A	2331	C	C5-C6-N1	5.03	123.52	121.00
20	A	2781	C	C2-N1-C1'	5.03	124.34	118.80
1	a	1040	U	N3-C2-O2	-5.03	118.68	122.20
20	A	1531	G	N9-C4-C5	-5.03	103.39	105.40
20	A	1591	A	C8-N9-C1'	-5.03	118.65	127.70
21	B	35	C	C2-N1-C1'	5.03	124.33	118.80
20	A	931	C	N1-C2-O2	5.02	121.91	118.90
1	a	221	C	C6-N1-C2	-5.02	118.29	120.30
20	A	1236	U	C2-N1-C1'	5.02	123.72	117.70
20	A	203	U	N3-C2-O2	-5.01	118.69	122.20
20	A	344	G	O4'-C1'-N9	5.01	112.21	108.20
20	A	2520	U	N3-C2-O2	-5.01	118.69	122.20
20	A	2303	G	C8-N9-C4	-5.01	104.39	106.40
20	A	1591	A	N3-C4-C5	-5.01	123.29	126.80
20	A	2162	G	N3-C4-N9	-5.01	122.99	126.00
20	A	2630	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1183	C	C2-N1-C1'	5.01	124.31	118.80
20	A	2534	C	N3-C2-O2	-5.01	118.40	121.90
20	A	2119	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	4	20	LYS	Peptide
47	4	3	ARG	Peptide
23	D	53	TYR	Peptide
23	D	89	GLY	Peptide
25	F	121	ALA	Peptide

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Mol	Chain	Res	Type	Group
26	G	46	GLU	Peptide
26	G	47	GLY	Peptide
29	M	30	THR	Peptide
29	M	85	PHE	Peptide
29	M	94	VAL	Peptide
29	M	97	LYS	Peptide
30	N	133	LYS	Peptide
30	N	8	LYS	Peptide
31	O	23	ASP	Peptide
32	P	30	ARG	Peptide
32	P	61	LYS	Peptide
34	R	88	ILE	Peptide
35	S	50	ALA	Peptide
36	T	26	ILE	Peptide
37	U	50	VAL	Peptide
38	V	72	ASP	Peptide
38	V	97	THR	Peptide
39	W	13	ARG	Peptide
40	X	49	GLN	Peptide
2	c	161	ILE	Peptide
3	d	189	GLU	Peptide
17	r	19	ALA	Peptide
17	r	26	ASP	Peptide
19	t	66	ILE	Peptide
19	t	68	LYS	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%)	177 (88%)	25 (12%)	0	100	100
3	d	199/201 (99%)	170 (85%)	29 (15%)	0	100	100
4	e	161/163 (99%)	148 (92%)	13 (8%)	0	100	100
5	f	95/97 (98%)	81 (85%)	14 (15%)	0	100	100
6	g	152/154 (99%)	137 (90%)	15 (10%)	0	100	100
7	h	129/131 (98%)	114 (88%)	15 (12%)	0	100	100
8	i	126/128 (98%)	113 (90%)	13 (10%)	0	100	100
9	j	97/99 (98%)	78 (80%)	19 (20%)	0	100	100
10	k	115/117 (98%)	93 (81%)	22 (19%)	0	100	100
11	l	134/136 (98%)	105 (78%)	28 (21%)	1 (1%)	22	61
12	m	110/112 (98%)	91 (83%)	19 (17%)	0	100	100
13	n	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
14	o	86/88 (98%)	74 (86%)	12 (14%)	0	100	100
15	p	87/89 (98%)	77 (88%)	10 (12%)	0	100	100
16	q	81/83 (98%)	65 (80%)	16 (20%)	0	100	100
17	r	64/66 (97%)	54 (84%)	10 (16%)	0	100	100
18	s	76/78 (97%)	64 (84%)	12 (16%)	0	100	100
19	t	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
22	C	271/275 (98%)	229 (84%)	42 (16%)	0	100	100
23	D	205/207 (99%)	167 (82%)	37 (18%)	1 (0%)	29	67
24	E	204/206 (99%)	170 (83%)	34 (17%)	0	100	100
25	F	175/177 (99%)	155 (89%)	20 (11%)	0	100	100
26	G	172/176 (98%)	148 (86%)	23 (13%)	1 (1%)	25	64
27	K	143/145 (99%)	122 (85%)	21 (15%)	0	100	100
28	L	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
29	M	142/146 (97%)	108 (76%)	31 (22%)	3 (2%)	7	38
30	N	139/141 (99%)	116 (84%)	23 (16%)	0	100	100
31	O	121/123 (98%)	93 (77%)	28 (23%)	0	100	100
32	P	115/117 (98%)	98 (85%)	17 (15%)	0	100	100
33	Q	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
34	R	110/118 (93%)	105 (96%)	5 (4%)	0	100	100
35	S	100/102 (98%)	86 (86%)	14 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	T	110/112 (98%)	93 (84%)	17 (16%)	0	100	100
37	U	85/89 (96%)	68 (80%)	16 (19%)	1 (1%)	13	49
38	V	99/101 (98%)	75 (76%)	22 (22%)	2 (2%)	7	40
39	W	90/94 (96%)	65 (72%)	24 (27%)	1 (1%)	14	51
40	X	74/76 (97%)	60 (81%)	14 (19%)	0	100	100
41	Y	52/54 (96%)	46 (88%)	6 (12%)	0	100	100
42	Z	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
43	0	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
44	1	58/60 (97%)	43 (74%)	15 (26%)	0	100	100
45	2	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
46	3	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
47	4	42/44 (96%)	36 (86%)	6 (14%)	0	100	100
48	5	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
49	6	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
All	All	5104/5212 (98%)	4340 (85%)	754 (15%)	10 (0%)	50	80

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	M	95	VAL
29	M	98	GLU
26	G	47	GLY
38	V	73	PRO
23	D	54	GLN
39	W	74	MET
11	I	39	ASN
37	U	50	VAL
38	V	72	ASP
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%)	175 (100%)	0	100	100
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%)	130 (99%)	1 (1%)	81	89
7	h	112/112 (100%)	112 (100%)	0	100	100
8	i	101/101 (100%)	98 (97%)	3 (3%)	41	63
9	j	90/90 (100%)	88 (98%)	2 (2%)	52	70
10	k	91/91 (100%)	91 (100%)	0	100	100
11	l	118/118 (100%)	116 (98%)	2 (2%)	60	78
12	m	95/95 (100%)	94 (99%)	1 (1%)	73	84
13	n	51/51 (100%)	50 (98%)	1 (2%)	55	73
14	o	78/78 (100%)	76 (97%)	2 (3%)	46	67
15	p	79/79 (100%)	77 (98%)	2 (2%)	47	68
16	q	76/76 (100%)	74 (97%)	2 (3%)	46	67
17	r	57/57 (100%)	54 (95%)	3 (5%)	22	50
18	s	68/68 (100%)	67 (98%)	1 (2%)	65	79
19	t	62/62 (100%)	61 (98%)	1 (2%)	62	79
22	C	225/225 (100%)	224 (100%)	1 (0%)	91	94
23	D	169/170 (99%)	167 (99%)	2 (1%)	71	83
24	E	172/172 (100%)	170 (99%)	2 (1%)	71	83
25	F	153/154 (99%)	153 (100%)	0	100	100
26	G	146/146 (100%)	146 (100%)	0	100	100
27	K	121/122 (99%)	121 (100%)	0	100	100
28	L	98/98 (100%)	98 (100%)	0	100	100
29	M	112/112 (100%)	112 (100%)	0	100	100
30	N	111/112 (99%)	109 (98%)	2 (2%)	59	76
31	O	105/105 (100%)	104 (99%)	1 (1%)	76	86
32	P	91/91 (100%)	91 (100%)	0	100	100
33	Q	97/97 (100%)	97 (100%)	0	100	100
34	R	88/94 (94%)	87 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	S	82/83 (99%)	82 (100%)	0	100	100
36	T	95/95 (100%)	95 (100%)	0	100	100
37	U	79/80 (99%)	79 (100%)	0	100	100
38	V	85/85 (100%)	85 (100%)	0	100	100
39	W	84/85 (99%)	84 (100%)	0	100	100
40	X	61/61 (100%)	61 (100%)	0	100	100
41	Y	47/47 (100%)	45 (96%)	2 (4%)	29	55
42	Z	55/55 (100%)	55 (100%)	0	100	100
43	0	49/49 (100%)	49 (100%)	0	100	100
44	1	55/55 (100%)	55 (100%)	0	100	100
45	2	46/46 (100%)	45 (98%)	1 (2%)	52	70
46	3	49/49 (100%)	49 (100%)	0	100	100
47	4	38/39 (97%)	38 (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	4357/4371 (100%)	4324 (99%)	33 (1%)	82	89

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	g	36	ARG
8	i	12	ARG
8	i	14	ASN
8	i	130	ARG
9	j	5	LYS
9	j	16	ARG
11	l	32	LYS
11	l	134	ARG
12	m	107	ARG
13	n	26	ARG
14	o	54	ARG
14	o	89	ARG
15	p	32	ARG
15	p	90	LYS
16	q	5	ARG
16	q	6	ASN
17	r	13	LYS

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Mol	Chain	Res	Type
17	r	57	ARG
17	r	65	ARG
18	s	6	LYS
19	t	81	LEU
22	C	257	TYR
23	D	119	PHE
23	D	168	ARG
24	E	74	ARG
24	E	169	ASN
30	N	10	ARG
30	N	74	TYR
31	O	65	PHE
34	R	94	MET
41	Y	17	ASN
41	Y	32	ASN
45	2	49	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
2	c	6	HIS
2	c	85	ASN
3	d	35	GLN
3	d	50	GLN
3	d	200	ASN
6	g	28	ASN
6	g	68	ASN
6	g	86	GLN
6	g	106	ASN
6	g	142	HIS
8	i	5	GLN
8	i	66	ASN
8	i	75	GLN
8	i	89	GLN
8	i	126	GLN
11	l	39	ASN
11	l	90	HIS
13	n	19	GLN
14	o	9	ASN
14	o	28	GLN
15	p	88	ASN
16	q	6	ASN

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Mol	Chain	Res	Type
16	q	54	ASN
17	r	21	HIS
17	r	56	GLN
18	s	22	GLN
19	t	67	HIS
19	t	69	ASN
19	t	72	ASN
22	C	134	ASN
22	C	177	ASN
22	C	197	ASN
22	C	232	HIS
23	D	50	GLN
24	E	49	HIS
24	E	67	GLN
24	E	75	GLN
24	E	158	ASN
24	E	169	ASN
25	F	27	GLN
25	F	37	ASN
25	F	178	GLN
26	G	6	ASN
26	G	147	ASN
32	P	32	ASN
34	R	29	HIS
35	S	101	ASN
36	T	65	ASN
37	U	57	ASN
40	X	87	GLN
41	Y	32	ASN
41	Y	34	GLN
43	0	40	ASN
43	0	48	ASN
45	2	32	ASN
46	3	4	ASN
47	4	8	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1528 (99%)	423 (27%)	0
20	A	2890/2903 (99%)	844 (29%)	24 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	B	115/116 (99%)	38 (33%)	0
All	All	4531/4547 (99%)	1305 (28%)	24 (0%)

All (1305) 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	18	G
1	a	19	G
1	a	20	C
1	a	28	G
1	a	29	A
1	a	36	G
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	56	A
1	a	60	C
1	a	62	A
1	a	65	G
1	a	72	U
1	a	74	C
1	a	75	U
1	a	97	G
1	a	103	A
1	a	114	A
1	a	117	G
1	a	124	A
1	a	125	A
1	a	126	C
1	a	127	A
1	a	135	A
1	a	136	A
1	a	138	C
1	a	162	U

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Mol	Chain	Res	Type
1	a	165	G
1	a	169	C
1	a	183	G
1	a	188	A
1	a	189	C
1	a	202	A
1	a	205	G
1	a	211	G
1	a	212	A
1	a	218	A
1	a	219	G
1	a	222	G
1	a	226	U
1	a	227	C
1	a	228	G
1	a	229	G
1	a	230	G
1	a	235	G
1	a	254	G
1	a	255	U
1	a	256	G
1	a	259	U
1	a	260	U
1	a	261	A
1	a	262	G
1	a	265	A
1	a	266	G
1	a	281	G
1	a	282	C
1	a	289	A
1	a	294	A
1	a	295	C
1	a	296	G
1	a	302	U
1	a	304	G
1	a	319	U
1	a	323	C
1	a	328	A
1	a	330	A
1	a	331	C
1	a	335	G
1	a	342	A

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Mol	Chain	Res	Type
1	a	343	C
1	a	359	A
1	a	361	G
1	a	362	G
1	a	367	C
1	a	369	G
1	a	375	G
1	a	378	A
1	a	382	U
1	a	383	U
1	a	387	C
1	a	388	A
1	a	393	A
1	a	399	G
1	a	405	C
1	a	407	G
1	a	412	A
1	a	413	C
1	a	421	G
1	a	426	A
1	a	427	A
1	a	428	G
1	a	429	A
1	a	430	A
1	a	433	U
1	a	436	U
1	a	439	G
1	a	443	G
1	a	444	U
1	a	453	G
1	a	454	U
1	a	455	U
1	a	463	A
1	a	464	A
1	a	476	U
1	a	478	A
1	a	479	G
1	a	483	C
1	a	484	U
1	a	485	G
1	a	486	A
1	a	488	C

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Mol	Chain	Res	Type
1	a	489	G
1	a	490	U
1	a	492	C
1	a	493	C
1	a	495	U
1	a	499	G
1	a	500	G
1	a	501	U
1	a	510	A
1	a	511	G
1	a	512	A
1	a	518	A
1	a	524	A
1	a	526	C
1	a	533	C
1	a	534	C
1	a	539	G
1	a	540	C
1	a	542	G
1	a	545	G
1	a	546	U
1	a	548	A
1	a	550	A
1	a	551	C
1	a	560	C
1	a	562	A
1	a	576	U
1	a	577	U
1	a	579	U
1	a	585	G
1	a	587	A
1	a	590	G
1	a	591	C
1	a	592	G
1	a	610	A
1	a	611	A
1	a	619	G
1	a	620	U
1	a	622	A
1	a	625	G
1	a	635	C
1	a	644	A

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Mol	Chain	Res	Type
1	a	648	U
1	a	656	A
1	a	668	U
1	a	670	A
1	a	680	A
1	a	683	A
1	a	690	A
1	a	701	U
1	a	703	G
1	a	716	U
1	a	729	G
1	a	732	C
1	a	733	A
1	a	736	A
1	a	738	U
1	a	744	A
1	a	746	G
1	a	749	G
1	a	753	U
1	a	757	G
1	a	761	G
1	a	763	A
1	a	764	A
1	a	768	A
1	a	770	G
1	a	807	A
1	a	808	U
1	a	814	G
1	a	820	C
1	a	831	A
1	a	832	C
1	a	833	G
1	a	834	A
1	a	836	G
1	a	840	G
1	a	843	A
1	a	847	G
1	a	857	U
1	a	858	U
1	a	859	C
1	a	860	C
1	a	861	G

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Mol	Chain	Res	Type
1	a	862	C
1	a	869	G
1	a	883	G
1	a	886	U
1	a	887	U
1	a	888	A
1	a	890	G
1	a	892	A
1	a	901	G
1	a	905	A
1	a	906	G
1	a	927	U
1	a	929	A
1	a	930	A
1	a	939	A
1	a	942	G
1	a	943	G
1	a	944	G
1	a	946	C
1	a	950	C
1	a	951	A
1	a	952	C
1	a	955	G
1	a	959	U
1	a	974	A
1	a	976	U
1	a	977	U
1	a	978	C
1	a	981	A
1	a	982	G
1	a	985	A
1	a	987	G
1	a	988	C
1	a	990	A
1	a	991	A
1	a	992	G
1	a	993	A
1	a	998	U
1	a	999	A
1	a	1007	U
1	a	1008	U
1	a	1009	G

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Mol	Chain	Res	Type
1	a	1010	A
1	a	1012	A
1	a	1013	U
1	a	1018	U
1	a	1020	A
1	a	1025	U
1	a	1030	A
1	a	1031	G
1	a	1033	U
1	a	1034	A
1	a	1036	A
1	a	1039	U
1	a	1040	U
1	a	1041	U
1	a	1043	C
1	a	1044	C
1	a	1045	U
1	a	1047	C
1	a	1048	G
1	a	1052	A
1	a	1053	C
1	a	1054	A
1	a	1056	A
1	a	1057	G
1	a	1060	A
1	a	1061	C
1	a	1066	G
1	a	1069	G
1	a	1072	U
1	a	1077	G
1	a	1080	G
1	a	1081	U
1	a	1082	C
1	a	1092	C
1	a	1097	G
1	a	1100	G
1	a	1101	U
1	a	1102	U
1	a	1103	G
1	a	1107	U
1	a	1109	A
1	a	1110	G

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Mol	Chain	Res	Type
1	a	1111	U
1	a	1113	C
1	a	1117	A
1	a	1120	G
1	a	1124	G
1	a	1134	U
1	a	1139	A
1	a	1140	G
1	a	1141	U
1	a	1143	G
1	a	1144	C
1	a	1145	C
1	a	1146	A
1	a	1148	C
1	a	1154	G
1	a	1155	U
1	a	1156	U
1	a	1157	G
1	a	1161	A
1	a	1162	C
1	a	1167	G
1	a	1169	G
1	a	1170	A
1	a	1172	A
1	a	1173	C
1	a	1174	U
1	a	1182	A
1	a	1184	A
1	a	1197	G
1	a	1199	G
1	a	1200	G
1	a	1201	G
1	a	1205	G
1	a	1211	A
1	a	1212	A
1	a	1213	A
1	a	1216	A
1	a	1218	C
1	a	1227	U
1	a	1228	A
1	a	1229	U
1	a	1231	A

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Mol	Chain	Res	Type
1	a	1237	G
1	a	1239	U
1	a	1240	A
1	a	1241	C
1	a	1242	A
1	a	1253	A
1	a	1254	A
1	a	1255	U
1	a	1256	G
1	a	1257	G
1	a	1262	U
1	a	1263	A
1	a	1268	G
1	a	1271	U
1	a	1272	C
1	a	1273	G
1	a	1274	C
1	a	1275	U
1	a	1276	A
1	a	1283	G
1	a	1286	G
1	a	1288	C
1	a	1289	A
1	a	1290	U
1	a	1294	A
1	a	1295	A
1	a	1296	U
1	a	1297	C
1	a	1302	A
1	a	1303	A
1	a	1305	G
1	a	1307	U
1	a	1309	C
1	a	1312	U
1	a	1313	C
1	a	1314	A
1	a	1315	G
1	a	1317	U
1	a	1318	C
1	a	1320	G
1	a	1324	G
1	a	1332	C

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Mol	Chain	Res	Type
1	a	1335	C
1	a	1337	C
1	a	1345	U
1	a	1346	G
1	a	1347	A
1	a	1351	C
1	a	1360	U
1	a	1361	A
1	a	1362	G
1	a	1374	C
1	a	1375	A
1	a	1376	G
1	a	1384	C
1	a	1386	G
1	a	1390	A
1	a	1393	C
1	a	1396	U
1	a	1397	C
1	a	1402	G
1	a	1403	C
1	a	1405	U
1	a	1406	U
1	a	1410	C
1	a	1412	C
1	a	1416	G
1	a	1433	A
1	a	1434	G
1	a	1438	G
1	a	1440	A
1	a	1441	A
1	a	1457	A
1	a	1461	A
1	a	1465	U
1	a	1466	U
1	a	1467	U
1	a	1490	G
1	a	1496	A
1	a	1500	U
1	a	1503	G
1	a	1508	A
1	a	1509	A
1	a	1510	G

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Mol	Chain	Res	Type
1	a	1513	G
1	a	1515	A
1	a	1516	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
20	A	10	G
20	A	11	A
20	A	14	A
20	A	15	A
20	A	16	G
20	A	25	G
20	A	28	G
20	A	35	U
20	A	43	G
20	A	49	G
20	A	50	A
20	A	51	U
20	A	52	G
20	A	61	G
20	A	62	A
20	A	64	U
20	A	72	A
20	A	75	U
20	A	76	G
20	A	84	G
20	A	86	G
20	A	89	G
20	A	90	U
20	A	92	A
20	A	96	A
20	A	97	G
20	A	99	U
20	A	102	G
20	A	103	A
20	A	114	U
20	A	117	G
20	A	118	A
20	A	119	A

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Mol	Chain	Res	Type
20	A	120	U
20	A	131	A
20	A	134	A
20	A	143	A
20	A	151	A
20	A	155	U
20	A	156	U
20	A	162	A
20	A	163	A
20	A	164	U
20	A	165	A
20	A	166	C
20	A	168	U
20	A	169	A
20	A	170	G
20	A	171	C
20	A	180	G
20	A	182	U
20	A	189	A
20	A	199	A
20	A	202	A
20	A	207	A
20	A	218	G
20	A	219	A
20	A	224	A
20	A	226	A
20	A	231	A
20	A	233	U
20	A	234	C
20	A	235	G
20	A	236	A
20	A	242	U
20	A	244	A
20	A	250	G
20	A	251	G
20	A	253	G
20	A	254	A
20	A	255	G
20	A	258	A
20	A	268	A
20	A	270	C
20	A	272	C

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Mol	Chain	Res	Type
20	A	279	A
20	A	284	C
20	A	285	U
20	A	286	U
20	A	287	G
20	A	288	C
20	A	293	U
20	A	294	G
20	A	297	G
20	A	298	U
20	A	299	U
20	A	300	G
20	A	310	G
20	A	312	U
20	A	313	A
20	A	316	G
20	A	318	A
20	A	321	C
20	A	322	U
20	A	324	U
20	A	326	A
20	A	332	G
20	A	339	G
20	A	345	G
20	A	347	A
20	A	352	C
20	A	354	G
20	A	359	A
20	A	367	A
20	A	369	A
20	A	370	G
20	A	375	G
20	A	383	A
20	A	390	A
20	A	391	C
20	A	393	A
20	A	395	A
20	A	396	C
20	A	399	A
20	A	403	G
20	A	404	G
20	A	410	G

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Mol	Chain	Res	Type
20	A	414	A
20	A	421	A
20	A	422	A
20	A	426	G
20	A	430	A
20	A	446	G
20	A	451	G
20	A	462	A
20	A	471	U
20	A	484	C
20	A	487	A
20	A	489	A
20	A	494	A
20	A	496	C
20	A	504	U
20	A	506	A
20	A	507	G
20	A	508	G
20	A	509	G
20	A	517	A
20	A	519	A
20	A	521	G
20	A	523	A
20	A	533	G
20	A	543	U
20	A	544	A
20	A	547	U
20	A	548	C
20	A	549	C
20	A	551	G
20	A	554	A
20	A	561	G
20	A	565	A
20	A	566	C
20	A	567	A
20	A	568	A
20	A	569	C
20	A	570	A
20	A	571	A
20	A	572	G
20	A	576	A
20	A	585	A

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Mol	Chain	Res	Type
20	A	586	A
20	A	588	G
20	A	592	G
20	A	595	G
20	A	600	G
20	A	607	G
20	A	608	U
20	A	610	G
20	A	612	A
20	A	623	A
20	A	640	A
20	A	644	U
20	A	653	G
20	A	654	A
20	A	655	G
20	A	673	G
20	A	675	G
20	A	676	A
20	A	677	G
20	A	682	A
20	A	684	U
20	A	693	U
20	A	694	G
20	A	695	A
20	A	698	A
20	A	708	A
20	A	709	G
20	A	710	A
20	A	711	C
20	A	712	C
20	A	714	G
20	A	715	A
20	A	716	A
20	A	721	U
20	A	722	G
20	A	725	A
20	A	726	U
20	A	739	A
20	A	740	G
20	A	741	G
20	A	756	A
20	A	757	A

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Mol	Chain	Res	Type
20	A	758	A
20	A	759	C
20	A	762	A
20	A	766	G
20	A	767	A
20	A	769	G
20	A	770	A
20	A	774	A
20	A	776	C
20	A	785	G
20	A	786	U
20	A	787	U
20	A	791	A
20	A	792	A
20	A	801	A
20	A	802	U
20	A	803	G
20	A	804	A
20	A	805	G
20	A	808	G
20	A	814	A
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	825	U
20	A	828	A
20	A	830	A
20	A	832	G
20	A	833	A
20	A	834	A
20	A	837	U
20	A	840	A
20	A	842	A
20	A	845	G
20	A	846	C
20	A	851	U
20	A	852	C
20	A	867	U
20	A	868	U

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Mol	Chain	Res	Type
20	A	870	G
20	A	874	U
20	A	886	U
20	A	887	G
20	A	888	A
20	A	891	A
20	A	900	G
20	A	901	U
20	A	904	A
20	A	905	G
20	A	906	C
20	A	907	A
20	A	910	G
20	A	912	U
20	A	914	G
20	A	917	C
20	A	919	A
20	A	920	G
20	A	925	C
20	A	927	A
20	A	928	U
20	A	932	G
20	A	934	G
20	A	935	U
20	A	936	U
20	A	939	C
20	A	941	A
20	A	942	A
20	A	943	U
20	A	945	C
20	A	948	A
20	A	949	U
20	A	950	A
20	A	951	A
20	A	953	C
20	A	958	A
20	A	960	U
20	A	961	G
20	A	964	A
20	A	966	U
20	A	979	G
20	A	985	A

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Mol	Chain	Res	Type
20	A	986	G
20	A	993	A
20	A	996	G
20	A	997	A
20	A	998	U
20	A	999	A
20	A	1001	G
20	A	1014	A
20	A	1016	G
20	A	1020	A
20	A	1023	A
20	A	1025	C
20	A	1029	G
20	A	1036	A
20	A	1047	C
20	A	1049	A
20	A	1051	A
20	A	1052	U
20	A	1053	A
20	A	1060	A
20	A	1061	A
20	A	1062	G
20	A	1063	U
20	A	1066	A
20	A	1073	U
20	A	1081	U
20	A	1084	A
20	A	1086	A
20	A	1087	G
20	A	1088	A
20	A	1089	C
20	A	1092	C
20	A	1093	U
20	A	1095	G
20	A	1096	G
20	A	1097	A
20	A	1098	U
20	A	1100	U
20	A	1101	U
20	A	1102	G
20	A	1104	C
20	A	1105	U

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Mol	Chain	Res	Type
20	A	1108	G
20	A	1109	A
20	A	1110	A
20	A	1111	G
20	A	1112	C
20	A	1113	A
20	A	1114	G
20	A	1115	C
20	A	1116	C
20	A	1117	A
20	A	1118	C
20	A	1120	A
20	A	1122	U
20	A	1124	A
20	A	1125	A
20	A	1127	G
20	A	1128	A
20	A	1129	G
20	A	1131	G
20	A	1132	C
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	1145	U
20	A	1146	A
20	A	1148	U
20	A	1151	A
20	A	1152	G
20	A	1154	G
20	A	1156	C
20	A	1162	G
20	A	1166	A
20	A	1167	A
20	A	1168	A
20	A	1171	G

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Mol	Chain	Res	Type
20	A	1172	U
20	A	1174	C
20	A	1175	C
20	A	1176	G
20	A	1179	G
20	A	1181	U
20	A	1182	A
20	A	1195	A
20	A	1198	C
20	A	1209	A
20	A	1210	C
20	A	1212	A
20	A	1214	U
20	A	1215	A
20	A	1216	G
20	A	1217	G
20	A	1218	U
20	A	1219	G
20	A	1220	U
20	A	1247	U
20	A	1248	U
20	A	1257	A
20	A	1258	U
20	A	1265	G
20	A	1266	A
20	A	1271	U
20	A	1272	G
20	A	1273	G
20	A	1274	A
20	A	1275	G
20	A	1277	G
20	A	1284	A
20	A	1285	G
20	A	1290	A
20	A	1292	U
20	A	1293	G
20	A	1294	C
20	A	1302	A
20	A	1308	G
20	A	1309	A
20	A	1310	A
20	A	1311	A

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Mol	Chain	Res	Type
20	A	1335	G
20	A	1336	U
20	A	1337	A
20	A	1347	U
20	A	1350	C
20	A	1359	G
20	A	1365	U
20	A	1368	G
20	A	1369	C
20	A	1373	G
20	A	1376	U
20	A	1377	U
20	A	1378	A
20	A	1386	C
20	A	1396	G
20	A	1397	G
20	A	1401	A
20	A	1404	G
20	A	1410	G
20	A	1411	G
20	A	1414	A
20	A	1415	U
20	A	1417	G
20	A	1419	C
20	A	1420	A
20	A	1421	A
20	A	1428	G
20	A	1429	A
20	A	1431	A
20	A	1432	U
20	A	1436	U
20	A	1439	A
20	A	1443	G
20	A	1445	U
20	A	1446	G
20	A	1447	U
20	A	1448	U
20	A	1449	U
20	A	1450	U
20	A	1451	U
20	A	1452	G
20	A	1453	U

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Mol	Chain	Res	Type
20	A	1454	U
20	A	1455	U
20	A	1456	G
20	A	1457	A
20	A	1458	G
20	A	1461	A
20	A	1462	U
20	A	1463	G
20	A	1469	A
20	A	1470	C
20	A	1475	U
20	A	1479	C
20	A	1488	G
20	A	1489	C
20	A	1491	U
20	A	1492	G
20	A	1493	C
20	A	1494	G
20	A	1495	A
20	A	1496	U
20	A	1497	U
20	A	1500	A
20	A	1501	A
20	A	1503	U
20	A	1504	G
20	A	1507	U
20	A	1508	G
20	A	1509	U
20	A	1510	C
20	A	1512	A
20	A	1519	G
20	A	1521	G
20	A	1525	U
20	A	1530	A
20	A	1531	G
20	A	1532	A
20	A	1533	G
20	A	1536	A
20	A	1539	U
20	A	1545	A
20	A	1551	U
20	A	1552	A

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Mol	Chain	Res	Type
20	A	1559	A
20	A	1560	G
20	A	1561	U
20	A	1566	A
20	A	1567	C
20	A	1568	G
20	A	1573	G
20	A	1574	C
20	A	1576	A
20	A	1577	A
20	A	1584	G
20	A	1585	U
20	A	1586	A
20	A	1590	A
20	A	1592	G
20	A	1593	U
20	A	1599	A
20	A	1600	C
20	A	1601	G
20	A	1604	A
20	A	1605	C
20	A	1606	A
20	A	1612	A
20	A	1613	A
20	A	1615	A
20	A	1623	C
20	A	1624	U
20	A	1626	G
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	1650	U
20	A	1651	A
20	A	1652	A
20	A	1653	A
20	A	1665	A
20	A	1674	G
20	A	1677	U
20	A	1683	A

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Mol	Chain	Res	Type
20	A	1689	A
20	A	1690	G
20	A	1691	C
20	A	1697	A
20	A	1708	A
20	A	1711	A
20	A	1717	G
20	A	1718	C
20	A	1720	A
20	A	1723	U
20	A	1730	G
20	A	1741	A
20	A	1746	G
20	A	1756	U
20	A	1757	U
20	A	1758	C
20	A	1760	G
20	A	1768	C
20	A	1769	A
20	A	1770	G
20	A	1771	U
20	A	1774	A
20	A	1776	A
20	A	1777	G
20	A	1778	G
20	A	1787	A
20	A	1788	C
20	A	1790	G
20	A	1795	U
20	A	1798	A
20	A	1813	G
20	A	1814	C
20	A	1821	G
20	A	1822	U
20	A	1823	A
20	A	1828	G
20	A	1829	A
20	A	1830	A
20	A	1831	G
20	A	1833	A
20	A	1843	A
20	A	1844	C

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Mol	Chain	Res	Type
20	A	1872	G
20	A	1879	U
20	A	1882	C
20	A	1886	G
20	A	1890	A
20	A	1892	G
20	A	1911	G
20	A	1913	A
20	A	1914	A
20	A	1917	G
20	A	1920	G
20	A	1925	U
20	A	1943	G
20	A	1944	G
20	A	1950	A
20	A	1952	A
20	A	1954	U
20	A	1963	G
20	A	1969	U
20	A	1970	U
20	A	1977	C
20	A	1978	G
20	A	1979	C
20	A	1980	A
20	A	1981	C
20	A	1983	A
20	A	1984	A
20	A	1985	A
20	A	1986	G
20	A	1996	U
20	A	2005	U
20	A	2006	G
20	A	2008	C
20	A	2011	A
20	A	2032	U
20	A	2034	A
20	A	2035	G
20	A	2036	U
20	A	2044	A
20	A	2045	A
20	A	2046	G
20	A	2047	A

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Mol	Chain	Res	Type
20	A	2048	U
20	A	2057	C
20	A	2058	C
20	A	2069	C
20	A	2070	G
20	A	2071	G
20	A	2074	A
20	A	2075	G
20	A	2082	U
20	A	2083	G
20	A	2084	G
20	A	2101	G
20	A	2106	U
20	A	2107	G
20	A	2114	U
20	A	2115	G
20	A	2116	U
20	A	2120	A
20	A	2123	U
20	A	2125	U
20	A	2126	A
20	A	2127	C
20	A	2128	A
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	2144	G
20	A	2145	A
20	A	2146	U
20	A	2147	G
20	A	2148	A
20	A	2149	G
20	A	2159	C
20	A	2160	U
20	A	2162	G
20	A	2173	G
20	A	2177	C
20	A	2179	G

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Mol	Chain	Res	Type
20	A	2180	G
20	A	2182	G
20	A	2183	G
20	A	2184	G
20	A	2186	U
20	A	2187	A
20	A	2192	C
20	A	2193	C
20	A	2198	G
20	A	2200	U
20	A	2206	C
20	A	2212	A
20	A	2213	A
20	A	2217	G
20	A	2218	C
20	A	2226	A
20	A	2227	U
20	A	2228	C
20	A	2234	G
20	A	2235	G
20	A	2239	A
20	A	2252	G
20	A	2253	G
20	A	2257	U
20	A	2259	U
20	A	2273	G
20	A	2276	U
20	A	2280	A
20	A	2281	A
20	A	2282	A
20	A	2283	A
20	A	2287	A
20	A	2292	A
20	A	2297	C
20	A	2298	C
20	A	2301	A
20	A	2302	A
20	A	2313	G
20	A	2318	G
20	A	2319	U
20	A	2321	G
20	A	2323	A

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Mol	Chain	Res	Type
20	A	2325	A
20	A	2326	U
20	A	2327	C
20	A	2333	A
20	A	2336	A
20	A	2339	G
20	A	2348	G
20	A	2349	A
20	A	2350	A
20	A	2359	G
20	A	2362	U
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	2399	C
20	A	2404	U
20	A	2405	G
20	A	2406	A
20	A	2407	U
20	A	2417	C
20	A	2419	G
20	A	2425	A
20	A	2436	C
20	A	2437	U
20	A	2439	A
20	A	2443	G
20	A	2444	A
20	A	2445	U
20	A	2453	A
20	A	2454	C
20	A	2455	C
20	A	2459	G
20	A	2461	G
20	A	2462	A
20	A	2466	C
20	A	2467	A
20	A	2482	A
20	A	2489	C

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Mol	Chain	Res	Type
20	A	2492	A
20	A	2497	C
20	A	2498	G
20	A	2504	G
20	A	2505	U
20	A	2508	G
20	A	2511	A
20	A	2515	C
20	A	2517	A
20	A	2518	U
20	A	2519	G
20	A	2521	C
20	A	2532	A
20	A	2534	C
20	A	2543	G
20	A	2548	C
20	A	2549	G
20	A	2561	U
20	A	2566	U
20	A	2570	C
20	A	2580	A
20	A	2581	G
20	A	2587	C
20	A	2590	G
20	A	2592	G
20	A	2595	G
20	A	2596	G
20	A	2597	G
20	A	2599	U
20	A	2600	C
20	A	2601	A
20	A	2616	A
20	A	2623	U
20	A	2624	C
20	A	2625	C
20	A	2627	U
20	A	2629	U
20	A	2635	G
20	A	2642	U
20	A	2643	U
20	A	2650	U
20	A	2660	C

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Mol	Chain	Res	Type
20	A	2661	U
20	A	2677	G
20	A	2696	G
20	A	2703	U
20	A	2728	G
20	A	2746	G
20	A	2747	A
20	A	2749	G
20	A	2753	U
20	A	2766	C
20	A	2770	U
20	A	2778	A
20	A	2779	A
20	A	2780	G
20	A	2790	A
20	A	2792	A
20	A	2793	U
20	A	2794	G
20	A	2795	A
20	A	2803	C
20	A	2804	A
20	A	2805	U
20	A	2806	U
20	A	2810	U
20	A	2811	U
20	A	2812	A
20	A	2813	A
20	A	2814	G
20	A	2818	G
20	A	2819	U
20	A	2828	U
20	A	2829	G
20	A	2832	A
20	A	2836	G
20	A	2841	G
20	A	2844	A
20	A	2845	G
20	A	2846	A
20	A	2848	A
20	A	2850	G
20	A	2854	G
20	A	2860	G

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Mol	Chain	Res	Type
20	A	2868	G
20	A	2877	G
20	A	2878	G
20	A	2880	G
20	A	2883	G
20	A	2891	C
20	A	2895	U
20	A	2897	G
20	A	2900	C
20	A	2902	A
20	A	2904	G
20	A	2910	A
20	A	2911	C
21	B	8	G
21	B	10	G
21	B	13	A
21	B	14	G
21	B	17	A
21	B	21	G
21	B	22	G
21	B	24	U
21	B	33	U
21	B	38	U
21	B	40	C
21	B	42	G
21	B	43	A
21	B	46	A
21	B	48	A
21	B	50	A
21	B	54	U
21	B	64	A
21	B	70	G
21	B	71	A
21	B	72	U
21	B	73	U
21	B	74	G
21	B	75	U
21	B	82	G
21	B	85	U
21	B	86	U
21	B	87	U
21	B	88	C

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Mol	Chain	Res	Type
21	B	91	U
21	B	92	U
21	B	94	G
21	B	95	U
21	B	97	A
21	B	100	G
21	B	101	U
21	B	102	A
21	B	107	G

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	179	A
20	A	311	A
20	A	312	U
20	A	427	A
20	A	654	A
20	A	693	U
20	A	890	A
20	A	960	U
20	A	963	C
20	A	1100	U
20	A	1138	A
20	A	1271	U
20	A	1431	A
20	A	1449	U
20	A	1530	A
20	A	1584	G
20	A	1585	U
20	A	1604	A
20	A	1605	C
20	A	2281	A
20	A	2317	G
20	A	2476	U
20	A	2658	A
20	A	2719	A

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	16.85
1	A	1579:U	O3'	1583:A	P	12.96
1	a	75:U	O3'	96:U	P	8.17

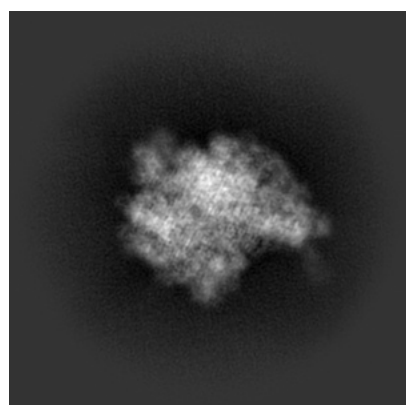
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0658. These allow visual inspection of the internal detail of the map and identification of artifacts.

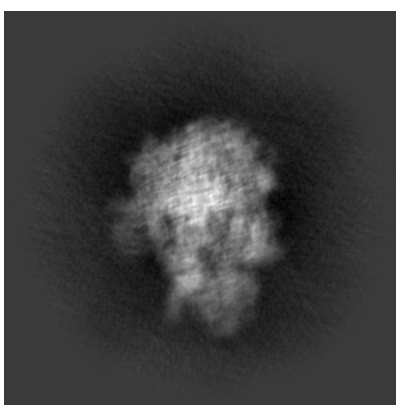
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

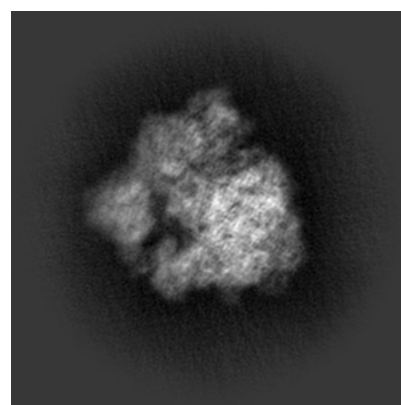
6.1.1 Primary map



X



Y

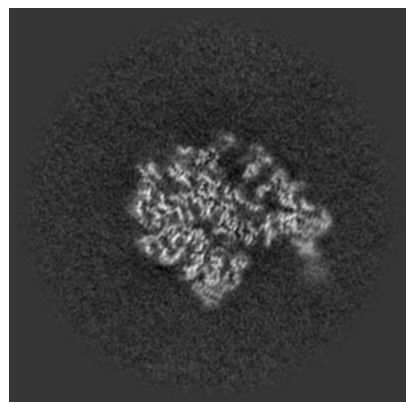


Z

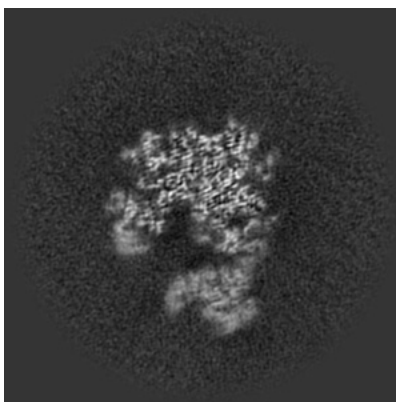
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

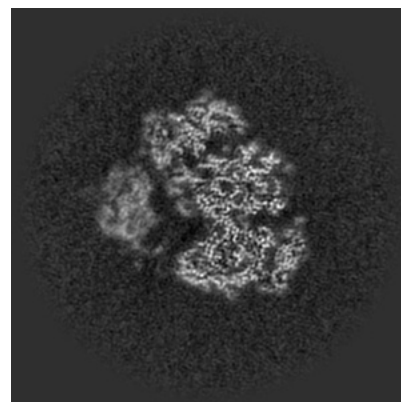
6.2.1 Primary map



X Index: 220



Y Index: 220

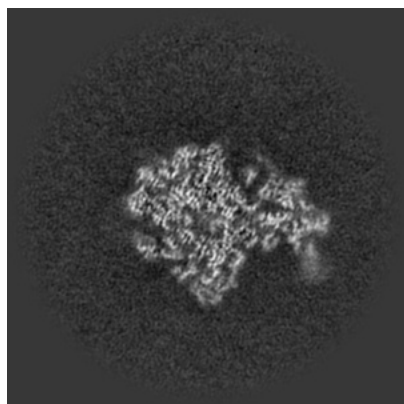


Z Index: 220

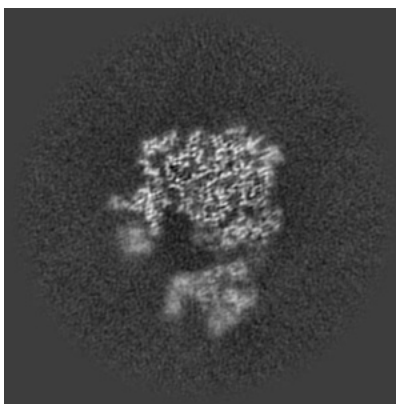
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

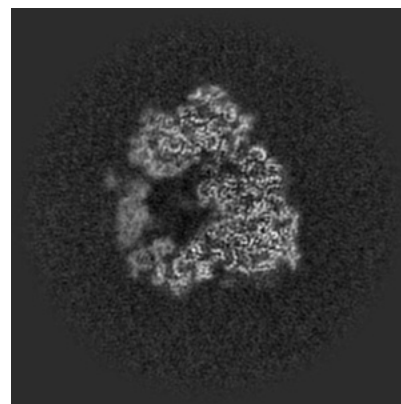
6.3.1 Primary map



X Index: 226



Y Index: 230

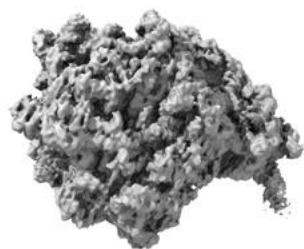


Z Index: 205

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.

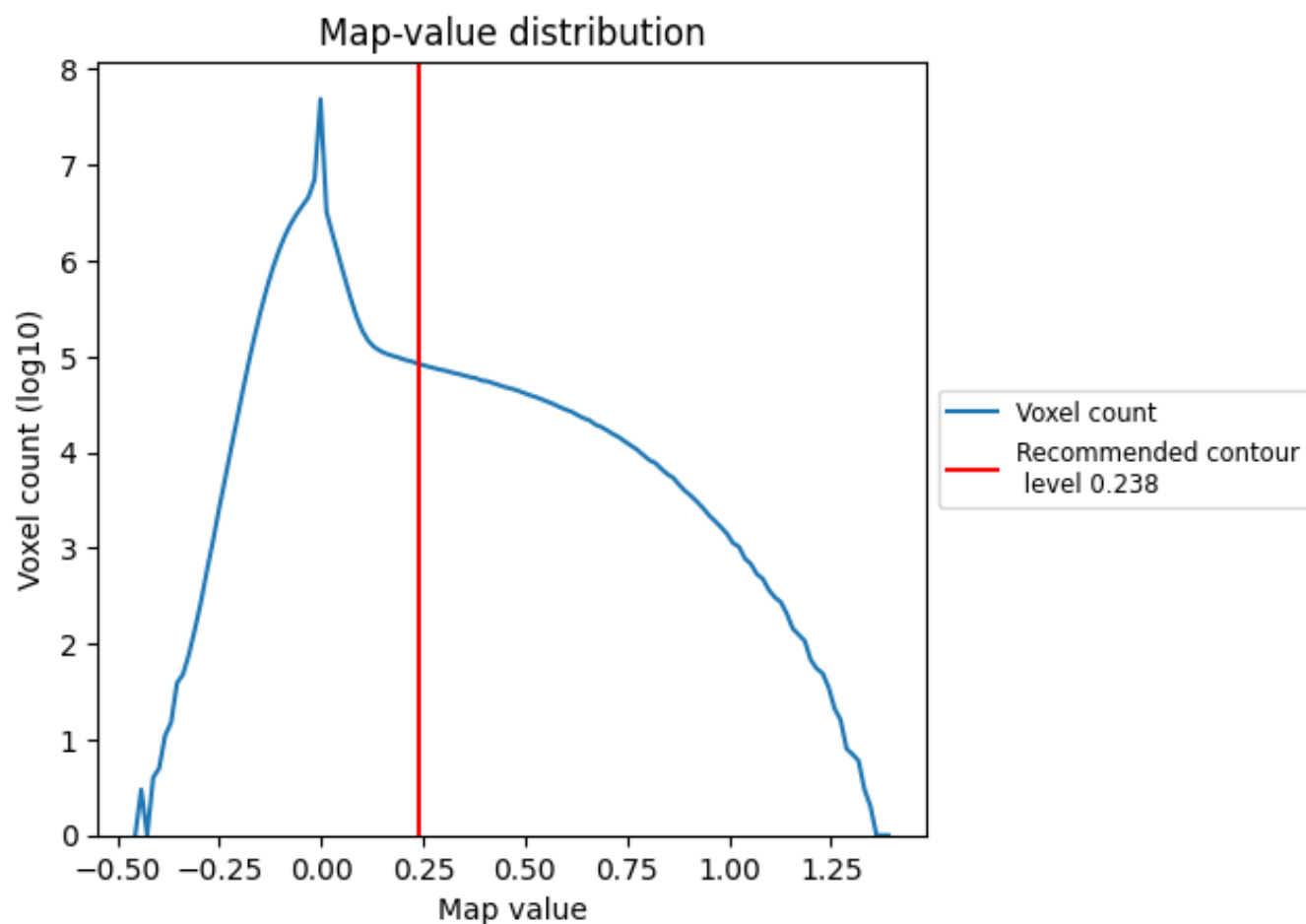
6.5 Mask visualisation

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

7 Map analysis [i](#)

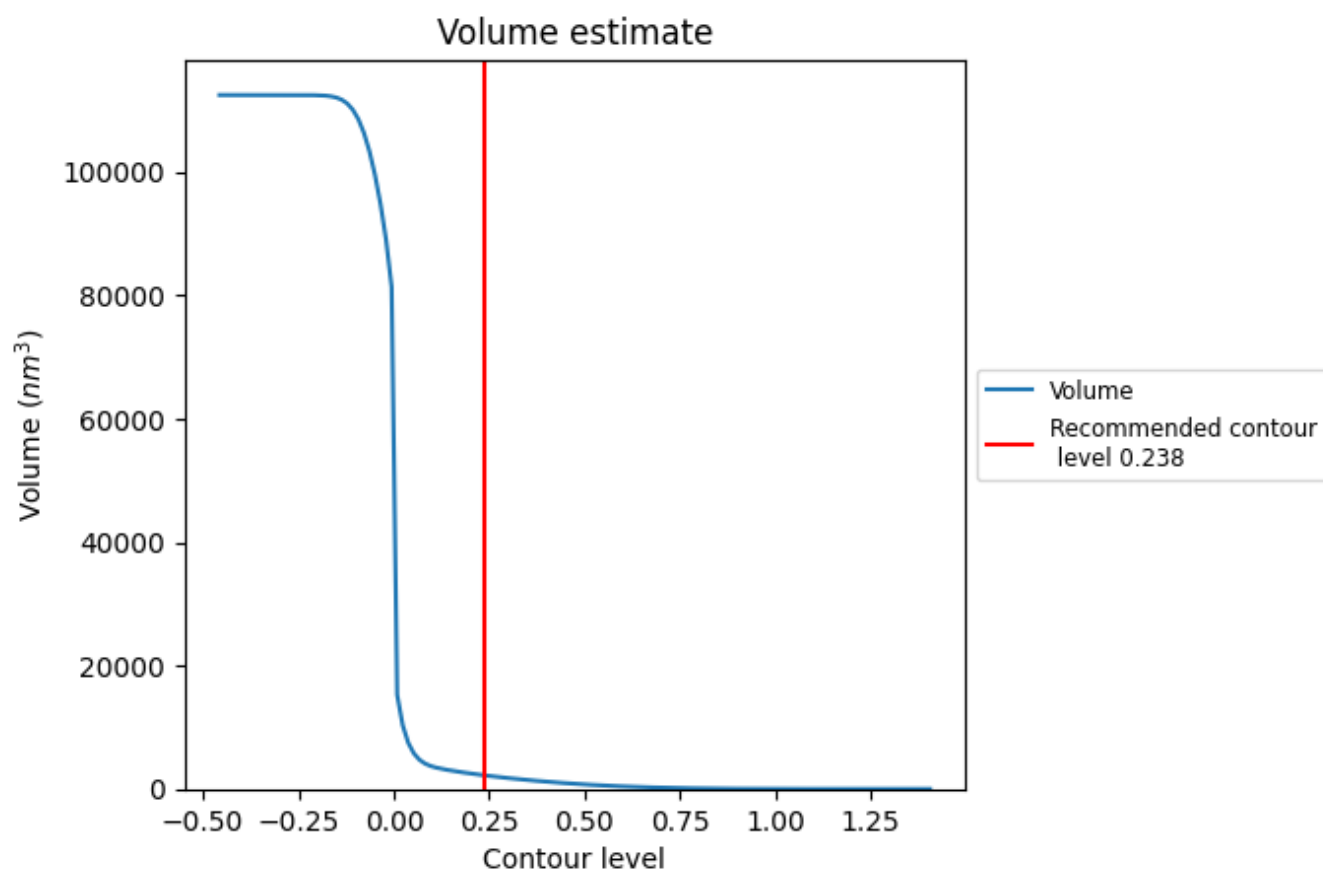
This section contains the results of statistical analysis of the map.

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.

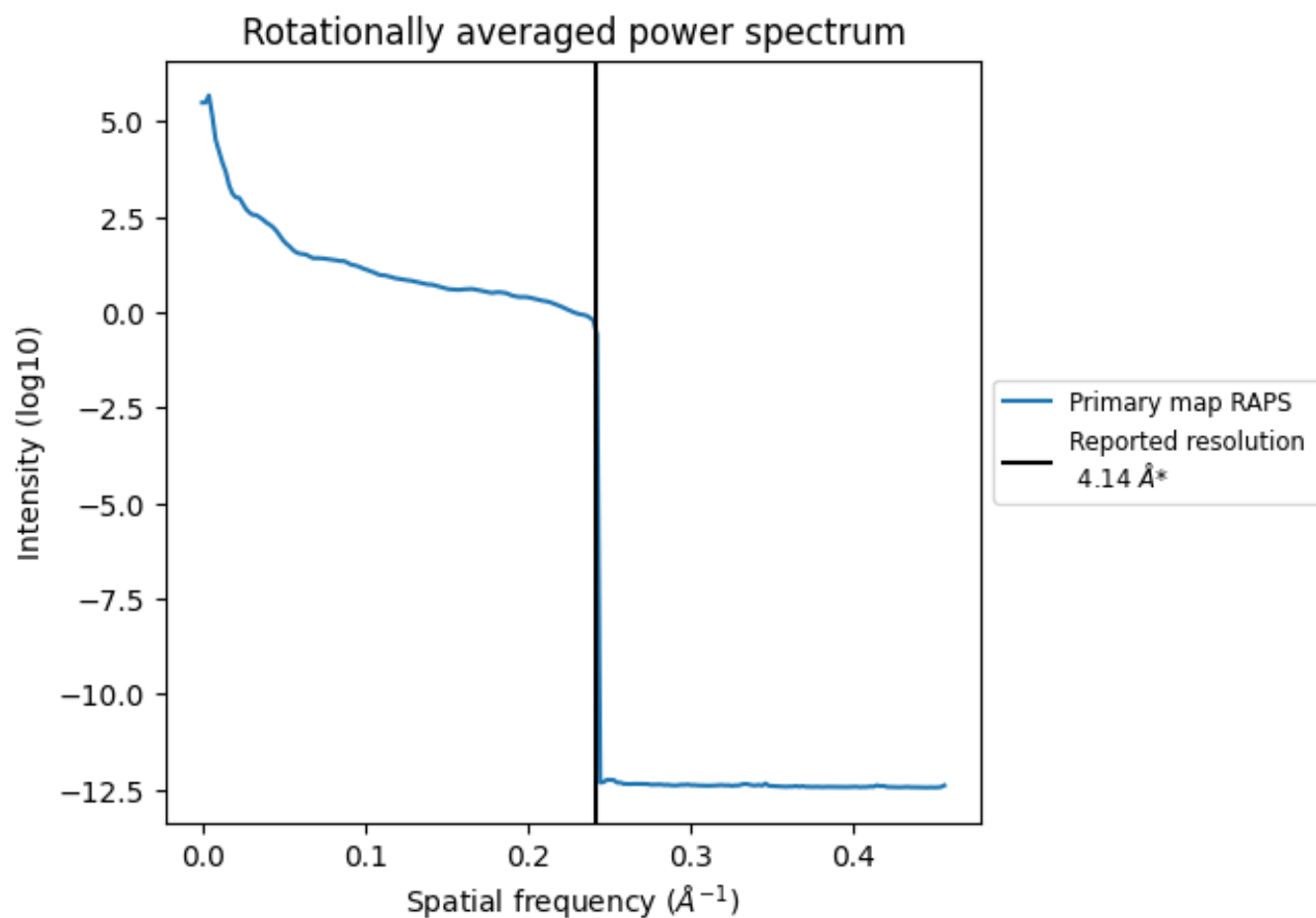
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2203 nm^3 ; this corresponds to an approximate mass of 1990 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 0.242 \AA^{-1}

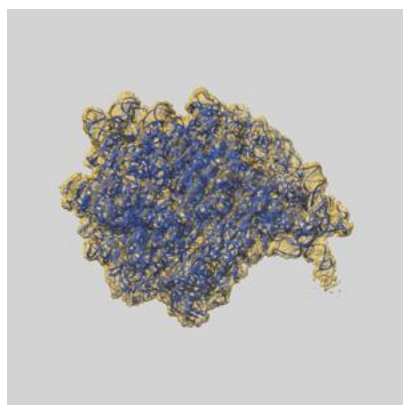
8 Fourier-Shell correlation ⓘ

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

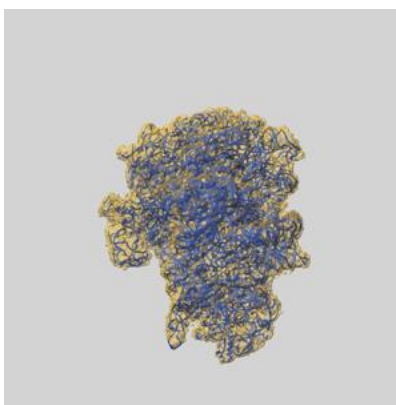
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0658 and PDB model 6O8Y. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

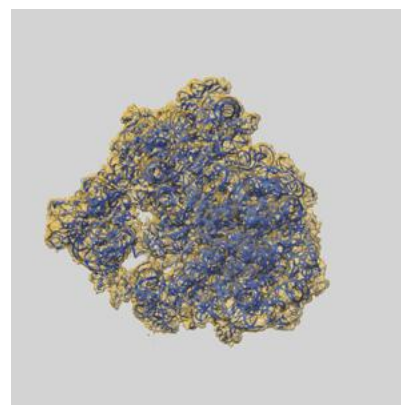
9.1 Map-model overlay [i](#)



X



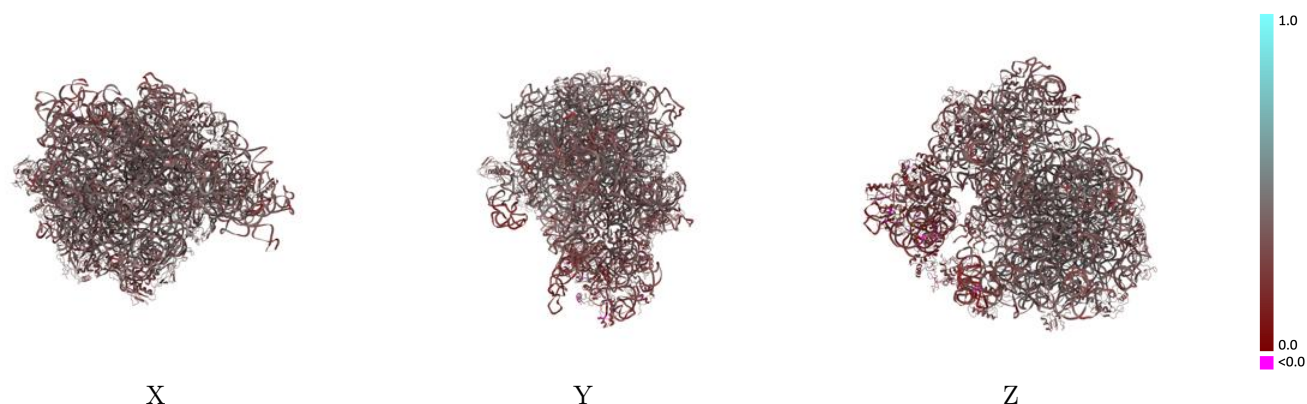
Y



Z

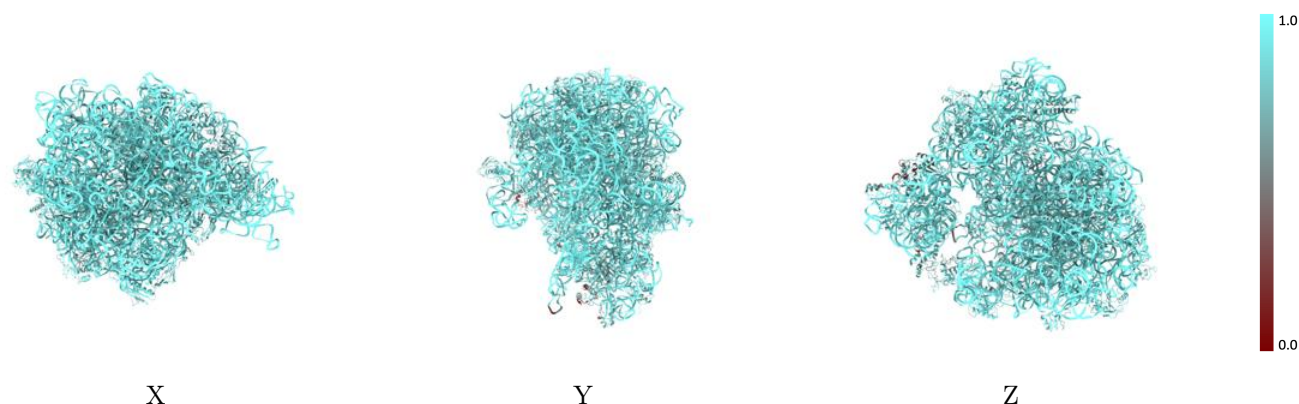
The images above show the 3D surface view of the map at the recommended contour level 0.238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



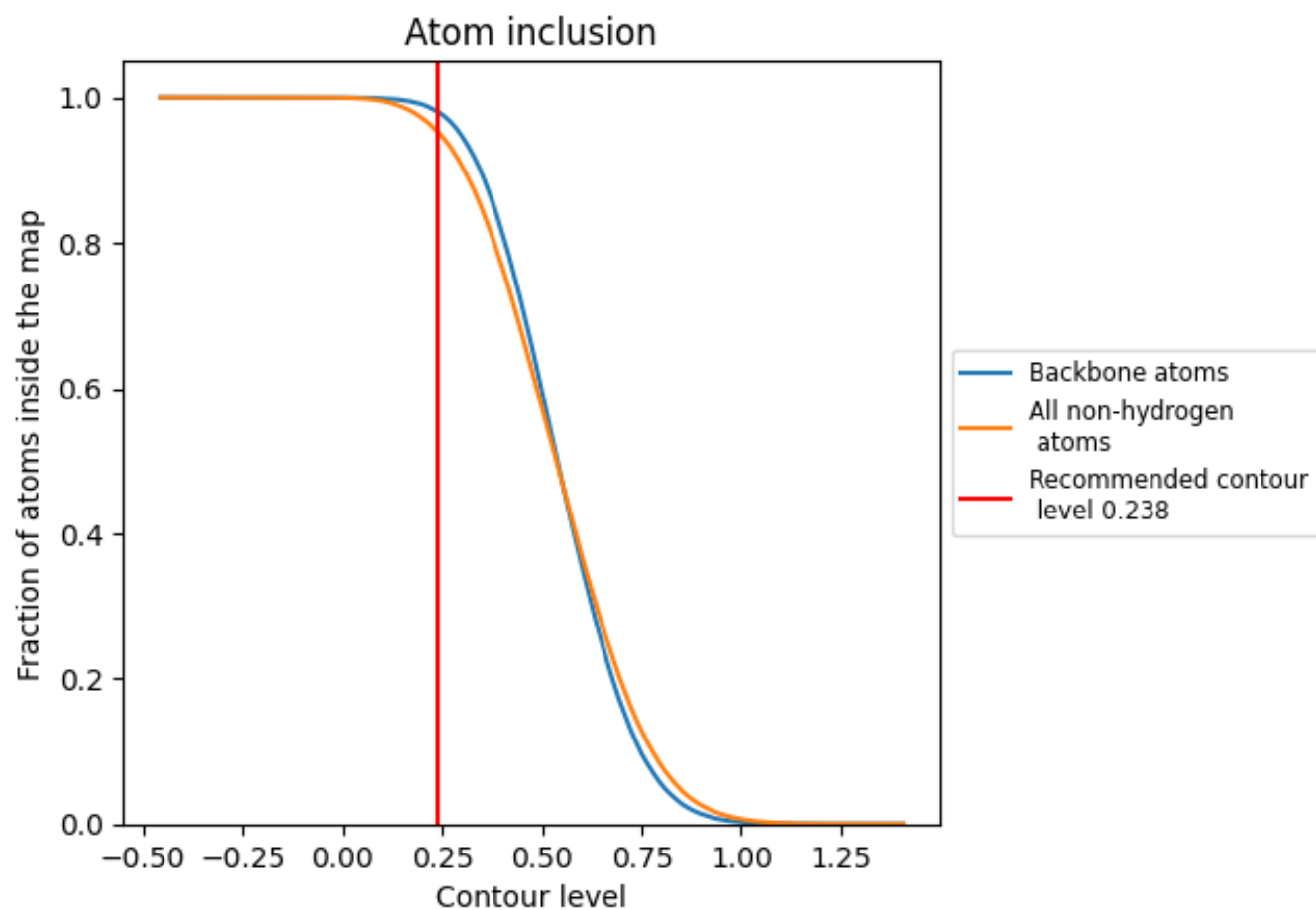
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% 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	 0.9540	 0.3450
0	 0.8811	 0.3710
1	 0.8443	 0.2370
2	 0.9429	 0.3970
3	 0.8960	 0.3450
4	 0.8800	 0.3650
5	 0.8632	 0.3710
6	 0.9356	 0.3490
A	 0.9914	 0.3680
B	 0.9931	 0.3230
C	 0.9033	 0.3850
D	 0.8729	 0.4030
E	 0.9025	 0.3600
F	 0.8316	 0.2500
G	 0.8856	 0.3290
K	 0.9058	 0.3820
L	 0.8473	 0.3990
M	 0.9130	 0.3770
N	 0.8209	 0.3520
O	 0.9205	 0.3640
P	 0.9118	 0.3040
Q	 0.8725	 0.3890
R	 0.9050	 0.3260
S	 0.9032	 0.3820
T	 0.9052	 0.3680
U	 0.9134	 0.3530
V	 0.8817	 0.3370
W	 0.3100	 0.2650
X	 0.9333	 0.3830
Y	 0.8592	 0.3670
Z	 0.9045	 0.3160
a	 0.9920	 0.3260
c	 0.7187	 0.2500
d	 0.8989	 0.2930
e	 0.8730	 0.3290



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Chain	Atom inclusion	Q-score
f	 0.8363	 0.3430
g	 0.8553	 0.2060
h	 0.8996	 0.3400
i	 0.8946	 0.2400
j	 0.8395	 0.2380
k	 0.8550	 0.3310
l	 0.8266	 0.3200
m	 0.7939	 0.1960
n	 0.9116	 0.2590
o	 0.8597	 0.3400
p	 0.9190	 0.3480
q	 0.8356	 0.3320
r	 0.8192	 0.3310
s	 0.8984	 0.1550
t	 0.8464	 0.2930