Full wwPDB X-ray Structure Validation Report (i)

May 23, 2024 – 05:23 PM EDT

PDB ID	:	4U3N
Title	:	Crystal structure of CCA trinucleotide bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-22
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 411288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	2	1750	37283	16668	6591	12274	1750	0	0	0
1	6	1795	38238	17095	6758	12590	1795	0	0	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S0	206	1577	1014	278	283	2	0	0	0
2	s0	206	1583	1017	281	283	2	0	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	S1	214	1709	1084	310	311	4	0	0	0
3	s1	216	1722	1091	312	315	4	0	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	S2	217	1635	1047	289	297	2	0	0	0
4	s2	217	1635	1047	289	297	2	0	0	0

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	S3	223	1734	1101	313	314	6	0	0	0
5	s3	223	1734	1101	313	314	6	0	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	S4	260	2068	1316	389	360	3	0	0	0
6	s4	260	2068	1316	389	360	3	0	0	0

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	S5	206	1609	1007	300	299	3	0	0	0
7	s5	206	1609	1007	300	299	3	0	0	0

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	S6	226	1799	1129	346	321	3	0	0	0
8	s6	218	1755	1102	337	313	3	0	0	0

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	S7	184	1481	951	265	265	0	0	0
9	s7	186	1491	957	267	267	0	0	0

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	S8	188	1489	925	298	264	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	s8	188	1489	925	298	264	2	0	0	0

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	S9	185	1494	943	289	261	1	0	0	0
			Total	C	N	O	S			
11	s9	185	1494	943	289	261	1	0	0	0

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	C0	96	773	500	126	145	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	C1	155	1214	775	230	206	3	0	0	0
			Total	C	N	O	S			
13	c1	146	1168	747	221	197	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47
c1	147	ALA	GLY	conflict	UNP P0CX47

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	C2	124	892	562	156	172	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	c2	124	892	562	156	172	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	104	ALA	GLY	conflict	UNP P48589
C2	110	ALA	GLY	conflict	UNP P48589
c2	104	ALA	GLY	conflict	UNP P48589
c2	110	ALA	GLY	conflict	UNP P48589

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	C3	150	1192	759	224	207	2	0	0	0
			Total	C	N	O	S			
15	c3	150	1192	759	224	207	2	0	0	0

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	C4	127	891	545	182	163	1	0	0	0
			Total	C	N	O	S			
16	c4	128	949	582	188	176	3	0	0	0

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	C5	124	977	622	182	166	7	0	0	0
			Total	C	N	O	S			
17	c5	135	1039	658	196	178	7	0	0	0

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	C6	141	1105	708	203	194	0	0	0
			Total	C	N	O			
18	c6	142	1111	711	204	196	0	0	0

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	C7	120	926	577	177	170	2	0	0	0
19	c7	117	906	563	174	167	2	0	0	0

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	C8	145	1192	743	237	210	2	0	0	0
20	c8	145	1192	743	237	210	2	0	0	0

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	C9	143	1112	694	208	208	2	0	0	0
21	c9	143	1112	694	208	208	2	0	0	0

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	D0	107	855	539	156	159	1	0	0	0
22	d0	110	882	554	161	166	1	0	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	D1	87	684	420	125	137	2	0	0	0
23	d1	87	684	420	125	137	2	0	0	0

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	D2	129	1021	650	188	180	3	0	0	0
24	d2	129	1021	650	188	180	3	0	0	0

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	D3	144	1121	708	220	191	2	0	0	0
25	d3	144	1121	708	220	191	2	0	0	0

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
26	D4	134	1073	676	208	189	0	0	0
26	d4	134	1073	676	208	189	0	0	0

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
27	D5	70	563	360	104	99	0	0	0
27	d5	69	558	357	103	98	0	0	0

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	D6	97	769	475	160	129	5	0	0	0
28	d6	97	769	475	160	129	5	0	0	0

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	D7	81	610	382	110	113	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	d7	81	610	382	110	113	5	0	0	0

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	D8	63	497	306	99	91	1	0	0	0
			Total	C	N	O	S			
30	d8	63	497	306	99	91	1	0	0	0

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	D9	53	442	274	92	72	4	0	0	0
			Total	C	N	O	S			
31	d9	53	442	274	92	72	4	0	0	0

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	E0	60	475	299	98	77	1	0	0	0

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	E1	71	566	362	106	94	4	0	0	0

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	SR	318	2441	1544	419	470	8	0	0	0
			Total	C	N	O	S			
34	sR	318	2442	1544	418	472	8	0	0	0

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	159	1104	652	221	231	0	0	0
35	sM	104	680	403	140	137	0	0	0

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	1	3149	67355	30086	12142	21978	3149	0	0	0
36	5	3150	67376	30095	12145	21987	3149	0	0	0

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
37	3	121	2579	1152	461	845	121	0	0	0
37	7	121	2579	1152	461	845	121	0	0	0

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
38	4	158	3353	1500	586	1109	158	0	0	0
38	8	158	3353	1500	586	1109	158	0	0	0

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	L2	252	1914	1191	388	334	1	0	0	0
39	l2	252	1912	1190	388	333	1	0	0	0

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L3	386	3075	1950	584	533	8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	l3	386	3075	1950	584	533	8	0	0	0

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	L4	361	2748	1729	522	494	3	0	0	0
			Total	C	N	O	S			
41	l4	361	2748	1729	522	494	3	0	0	0

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	L5	296	2375	1501	414	458	2	0	0	0
			Total	C	N	O	S			
42	l5	294	2359	1489	412	456	2	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	L6	156	1239	800	222	216	1	0	0	0
			Total	C	N	O	S			
43	l6	157	1248	806	224	217	1	0	0	0

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	L7	222	1784	1151	324	308	1	0	0	0
			Total	C	N	O	S			
44	l7	223	1791	1155	325	310	1	0	0	0

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L8	233	1804	1151	323	327	3	0	0	0
			Total	C	N	O	S			
45	l8	231	1763	1130	316	314	3	0	0	0

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	L9	191	1518	963	274	277	4	0	0	0
46	l9	191	1518	963	274	277	4	0	0	0

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	M0	211	1705	1083	322	294	6	0	0	0
47	m0	213	1722	1094	325	297	6	0	0	0

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	M1	169	1353	847	253	249	4	0	0	0
48	m1	169	1353	847	253	249	4	0	0	0

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	M3	193	1543	962	315	266	0	0	0
49	m3	194	1548	965	316	267	0	0	0

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	M4	136	1053	675	199	177	2	0	0	0
50	m4	137	1059	678	200	179	2	0	0	0

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	M5	203	1720	1077	361	281	1	0	0	0
51	m5	203	1720	1077	361	281	1	0	0	0

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	M6	197	1555	1003	289	262	1	0	0	0
52	m6	197	1555	1003	289	262	1	0	0	0

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
53	M7	183	1420	882	281	257	0	0	0
53	m7	155	1227	764	238	225	0	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	M8	185	1441	908	290	241	2	0	0	0
54	m8	185	1441	908	290	241	2	0	0	0

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
55	M9	188	1521	935	326	260	0	0	0
55	m9	188	1521	935	326	260	0	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	N0	172	1445	930	267	244	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	n0	172	1445	930	267	244	4	0	0	0

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	N1	159	1276	805	246	221	4	0	0	0
57	n1	159	1276	805	246	221	4	0	0	0

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
58	N2	100	796	516	131	149	0	0	0
58	n2	98	778	505	127	146	0	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	N3	136	1003	628	189	179	7	0	0	0
59	n3	136	1003	628	189	179	7	0	0	0

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
60	N4	98	699	443	137	118	1	0	0	0
60	n4	135	1038	651	206	180	1	0	0	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
61	N5	121	964	620	169	173	2	0	0	0
61	n5	120	959	617	168	172	2	0	0	0

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
62	N6	126	993	625	192	176	0	0	0
62	n6	126	993	625	192	176	0	0	0

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
63	N7	135	1092	710	202	180	0	0	0
63	n7	135	1092	710	202	180	0	0	0

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
64	N8	148	1173	749	231	190	3	0	0	0
64	n8	148	1173	749	231	190	3	0	0	0

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
65	N9	58	462	289	100	73	0	0	0
65	n9	58	462	289	100	73	0	0	0

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
66	O0	97	743	479	124	139	1	0	0	0
66	o0	100	767	492	128	146	1	0	0	0

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
67	O1	109	876	556	167	152	1	0	0	0
67	o1	109	883	559	167	156	1	0	0	0

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
68	O2	127	1020	647	205	167	1	0	0	0
68	o2	127	1020	647	205	167	1	0	0	0

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
69	O3	106	850	540	165	144	1	0	0	0
69	o3	106	850	540	165	144	1	0	0	0

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
70	O4	112	880	545	179	152	4	0	0	0
70	o4	112	880	545	179	152	4	0	0	0

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
71	O5	119	969	615	186	167	1	0	0	0
71	o5	119	965	612	185	167	1	0	0	0

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
72	O6	99	771	481	156	132	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
72	o6	99	770	481	156	131	2	0	0	0

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
73	O7	87	681	414	148	114	5	0	0	0
73	o7	87	681	414	148	114	5	0	0	0

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
74	O8	77	612	391	115	106	0	0	0
74	o8	77	608	388	114	106	0	0	0

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
75	O9	50	436	272	97	65	2	0	0	0
75	o9	50	436	272	97	65	2	0	0	0

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
76	Q0	52	417	259	86	67	5	0	0	0
76	q0	52	417	259	86	67	5	0	0	0

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
77	Q1	25	233	142	63	27	1	0	0	0
77	q1	25	233	142	63	27	1	0	0	0

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
78	Q2	105	847	534	170	138	5	0	0	0
78	q2	105	847	534	170	138	5	0	0	0

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
79	Q3	91	694	429	138	121	6	0	0	0
79	q3	91	694	429	138	121	6	0	0	0

- Molecule 80 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
80	c0	96	762	491	125	144	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c0	89	ALA	GLY	conflict	UNP Q08745

- Molecule 81 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	e0	62	491	309	101	80	1	0	0	0

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
82	e1	76	608	388	117	99	4	0	0	0

- Molecule 83 is a protein called UNKNOWN PROTEIN m2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
83	m2	150	750	450	150	150	0	0	0

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
84	p0	143	1077	687	192	195	3	0	0	0

- Molecule 85 is a protein called UNKNOWN PROTEIN p1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
85	p1	47	235	141	47	47	0	0	0

- Molecule 86 is a protein called UNKNOWN PROTEIN p2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
86	p2	46	230	138	46	46	0	0	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
87	2	124	124	124	0	0
87	S4	2	2	2	0	0
87	S8	1	1	1	0	0
87	D3	1	1	1	0	0
87	SM	1	1	1	0	0
87	1	477	477	477	0	0
87	3	14	14	14	0	0
87	4	19	19	19	0	0
87	L2	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
87	L3	3	3	3	0	0
87	L4	1	1	1	0	0
87	L5	1	1	1	0	0
87	L7	4	4	4	0	0
87	L8	1	1	1	0	0
87	M0	2	2	2	0	0
87	M1	1	1	1	0	0
87	M3	2	2	2	0	0
87	M5	2	2	2	0	0
87	M6	1	1	1	0	0
87	M7	4	4	4	0	0
87	M9	1	1	1	0	0
87	N0	1	1	1	0	0
87	N3	3	3	3	0	0
87	N5	1	1	1	0	0
87	N8	5	5	5	0	0
87	O2	1	1	1	0	0
87	O4	1	1	1	0	0
87	O5	1	1	1	0	0
87	O7	1	1	1	0	0
87	6	144	144	144	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
87	s1	1	1	1	0	0
87	s6	1	1	1	0	0
87	s8	3	3	3	0	0
87	c1	1	1	1	0	0
87	c7	2	2	2	0	0
87	c8	1	1	1	0	0
87	c9	1	1	1	0	0
87	d3	1	1	1	0	0
87	d4	1	1	1	0	0
87	d6	1	1	1	0	0
87	sM	1	1	1	0	0
87	5	502	502	502	0	0
87	7	15	15	15	0	0
87	8	16	16	16	0	0
87	l2	1	1	1	0	0
87	l3	3	3	3	0	0
87	l4	2	2	2	0	0
87	l5	2	2	2	0	0
87	l7	1	1	1	0	0
87	m1	2	2	2	0	0
87	m5	5	5	5	0	0

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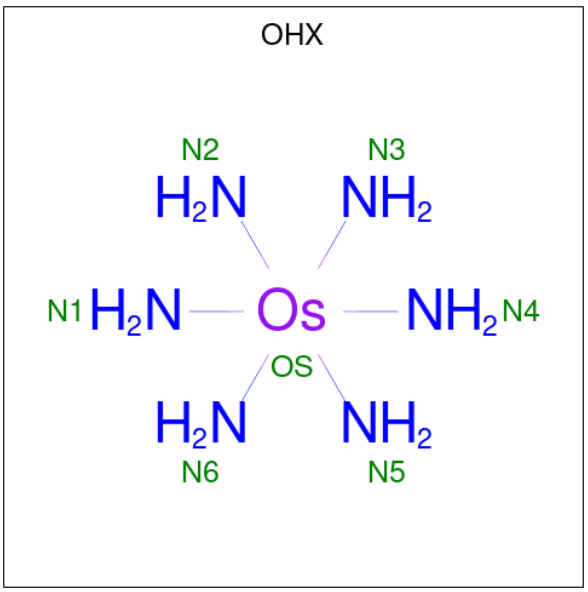
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
87	m6	2	2	2	0	0
87	m7	5	5	5	0	0
87	n0	3	3	3	0	0
87	n3	2	2	2	0	0
87	n6	2	2	2	0	0
87	n8	3	3	3	0	0
87	o1	1	1	1	0	0
87	o3	1	1	1	0	0
87	o4	1	1	1	0	0
87	q0	1	1	1	0	0
87	q1	1	1	1	0	0
87	q3	2	2	2	0	0

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
88	2	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	2	1	7	6	1	0	0
			Total	N	Os		
88	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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			Total	N	Os		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
88	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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			Total	N	Os		
88	2	1	7	6	1	0	0
			Total	N	Os		
88	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	2	1	7	6	1	0	0
			Total	N	Os		
88	2	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	2	1	7	6	1	0	0
			Total	N	Os		
88	2	1	7	6	1	0	0
			Total	N	Os		
88	S8	1	7	6	1	0	0
			Total	N	Os		
88	C3	1	7	6	1	0	0
			Total	N	Os		
88	C5	1	7	6	1	0	0
			Total	N	Os		
88	C8	1	7	6	1	0	0
			Total	N	Os		
88	D3	1	7	6	1	0	0
			Total	N	Os		
88	D9	1	7	6	1	0	0
			Total	N	Os		
88	SR	1	7	6	1	0	0
			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
88	1	1	7	6	1	0	0
			Total	N	Os		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	L3	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	M7	1	7	6	1	0	0
88	M7	1	7	6	1	0	0
88	M8	1	7	6	1	0	0
88	M9	1	7	6	1	0	0
88	N9	1	7	6	1	0	0
88	O3	1	7	6	1	0	0
88	O7	1	7	6	1	0	0
88	O7	1	7	6	1	0	0
88	6	1	7	6	1	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
88	s8	1	7	6	1	0	0
			Total	N	Os		
88	c1	1	7	6	1	0	0
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88	c3	1	7	6	1	0	0
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88	c5	1	7	6	1	0	0
			Total	N	Os		
88	c8	1	7	6	1	0	0
			Total	N	Os		
88	d4	1	7	6	1	0	0
			Total	N	Os		
88	d9	1	7	6	1	0	0
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88	sR	1	7	6	1	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
88	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
88	7	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
88	7	1	7	6	1	0	0
			Total	N	Os		
88	8	1	7	6	1	0	0
			Total	N	Os		
88	8	1	7	6	1	0	0
			Total	N	Os		
88	8	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
88	8	1	7	6	1	0	0
			Total	N	Os		
88	8	1	7	6	1	0	0
			Total	N	Os		
88	8	1	7	6	1	0	0
			Total	N	Os		
88	8	1	7	6	1	0	0
			Total	N	Os		
88	l3	1	7	6	1	0	0
			Total	N	Os		
88	l3	1	7	6	1	0	0
			Total	N	Os		
88	l3	1	7	6	1	0	0

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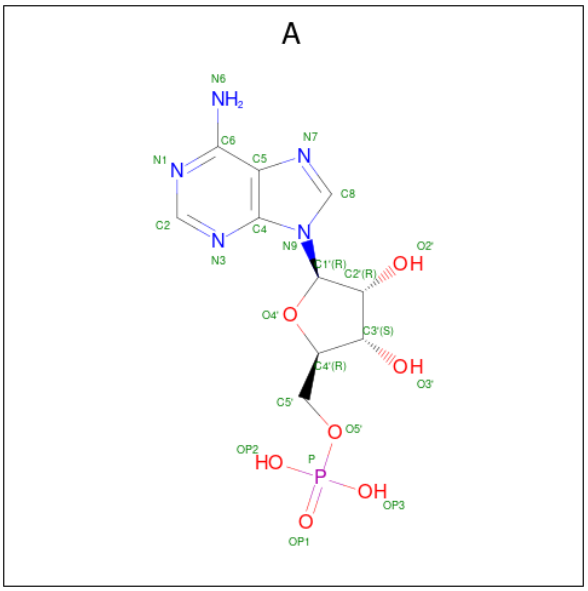
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	l4	1	7	6	1	0	0
88	l4	1	7	6	1	0	0
88	l5	1	7	6	1	0	0
88	l5	1	7	6	1	0	0
88	l5	1	7	6	1	0	0
88	l5	1	7	6	1	0	0
88	l9	1	7	6	1	0	0
88	m0	1	7	6	1	0	0
88	m0	1	7	6	1	0	0
88	m1	1	7	6	1	0	0
88	m4	1	7	6	1	0	0
88	m5	1	7	6	1	0	0
88	m6	1	7	6	1	0	0
88	n3	1	7	6	1	0	0
88	n3	1	7	6	1	0	0
88	n9	1	7	6	1	0	0
88	o3	1	7	6	1	0	0
88	o7	1	7	6	1	0	0
88	q2	1	7	6	1	0	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

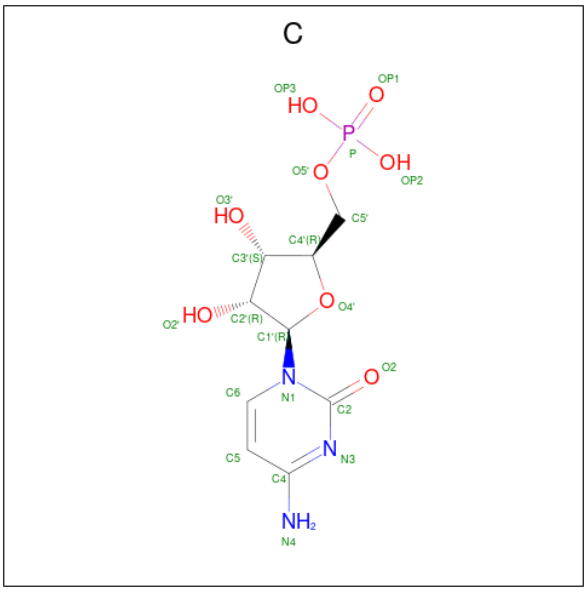
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
89	D6	1	1	1	0	0
89	D7	1	1	1	0	0
89	D9	1	1	1	0	0
89	E1	1	1	1	0	0
89	O7	1	1	1	0	0
89	Q0	1	1	1	0	0
89	Q2	1	1	1	0	0
89	Q3	1	1	1	0	0
89	d6	1	1	1	0	0
89	d7	1	1	1	0	0
89	d9	1	1	1	0	0
89	e1	1	1	1	0	0
89	o7	1	1	1	0	0
89	q0	1	1	1	0	0
89	q2	1	1	1	0	0
89	q3	1	1	1	0	0

- Molecule 90 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
90	1	1	22	10	5	6	1	0	0
			Total	C	N	O	P		
90	5	1	22	10	5	6	1	0	0

- Molecule 91 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
91	Q2	1	20	9	3	7	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
91	Q2	1	20	9	3	7	1	0	0
			Total	C	N	O	P		
91	q2	1	20	9	3	7	1	0	0
			Total	C	N	O	P		
91	q2	1	20	9	3	7	1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.02Å 287.59Å 304.52Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	49.82 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (49.82-3.20)	Depositor
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.181 , 0.237	Depositor
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.157	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411288	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 2563 ligands modelled in this entry, 1424 are monoatomic - leaving 1139 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.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.