Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:54 PM GMT

PDB ID : 4V9J

Title : 70S ribosome translocation intermediate GDPNP-II containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe*/E state.

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Deposited on : 2013-04-23

Resolution : 3.86 Å(reported)

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

MolProbity	:	NOT EXECUTED
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.86 Å.

There are no percentiles available for this entry.

MolProbity and EDS were not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 308202 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	235	Total 1910	C 1218	N 342	O 345	S 5	0	0	0
1	CB	235	Total 1910	C 1218	N 342	O 345	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	207	Total 1621	C 1022	N 315	O 283	S 1	0	0	0
2	CC	207	Total 1621	C 1022	N 315	O 283	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	208	Total 1703	C 1066	N 339	O 291	S 7	0	0	0
3	CD	208	Total 1703	C 1066	N 339	O 291	S 7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	151	Total 1156	C 729	N 218	O 205	S 4	0	0	0
4	CE	151	Total 1156	C 729	N 218	O 205	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	101	Total 843	C 531	N 155	O 154	S 3	0	0	0
5	CF	101	Total 843	C 531	N 155	O 154	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	155	Total 1257	C 781	N 252	O 218	S 6	0	0	0
6	CG	155	Total 1257	C 781	N 252	O 218	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	138	Total 1116	C 705	N 215	O 193	S 3	0	0	0
7	CH	138	Total 1116	C 705	N 215	O 193	S 3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AI	127	Total 1011	C 639	N 198	O 174	0	0	0
8	CI	127	Total 1011	C 639	N 198	O 174	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	99	Total 802	C 504	N 157	O 140	S 1	0	0	0
9	CJ	99	Total 802	C 504	N 157	O 140	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	119	Total 885	C 549	N 168	O 165	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			
11	CL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
12	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
13	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
14	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			
15	CP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	100	Total 835	C 534	N 156	O 143	S 2	0	0	0
16	CQ	100	Total 835	C 534	N 156	O 143	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	70	Total 574	C 367	N 112	O 95	0	0	0
17	CR	70	Total 574	C 367	N 112	O 95	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total 634	C 405	N 115	O 112	S 2	0	0	0
18	CS	79	Total 634	C 405	N 115	O 112	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	99	Total 762	C 469	N 162	O 129	S 2	0	0	0
19	CT	99	Total 762	C 469	N 162	O 129	S 2	0	0	0

• Molecule 20 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AA	1511	Total 32474	C 14455	N 6015	O 10494	P 1510	0	0	0
20	CA	1511	Total 32474	C 14455	N 6015	O 10494	P 1510	0	0	0

• Molecule 21 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	18	Total 393	C 177	N 81	O 118	P 17	0	0	0
21	CV	18	Total 393	C 177	N 81	O 118	P 17	0	0	0

- Molecule 22 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	77	Total 1635	C 732	N 291	O 536	P 76	0	0	0
22	CW	77	Total 1635	C 732	N 291	O 536	P 76	0	0	0

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	687	Total 5380	C 3414	N 922	O 1024	S 20	0	0	0
23	CY	687	Total 5380	C 3414	N 922	O 1024	S 20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	CONFLICT	UNP Q72I01
AY	226	ASN	HIS	CONFLICT	UNP Q72I01
CY	129	LYS	HIS	CONFLICT	UNP Q72I01
CY	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 24 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	6	Total 48	C 25	N 13	O 10	0	0	0
24	CU	6	Total 48	C 25	N 13	O 10	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	228	Total 1742	C 1101	N 319	O 319	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	20	VAL	ILE	CONFLICT	UNP Q72GV9
BC	28	ARG	HIS	CONFLICT	UNP Q72GV9
DC	20	VAL	ILE	CONFLICT	UNP Q72GV9
DC	28	ARG	HIS	CONFLICT	UNP Q72GV9

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
26	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			
27	DE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			
28	DF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	LYS	-	INSERTION	UNP Q72I05
BF	3	GLU	-	INSERTION	UNP Q72I05
BF	4	VAL	-	INSERTION	UNP Q72I05

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Chain	Residue	Modelled	Actual	Comment	Reference
BF	5	ALA	-	INSERTION	UNP Q72I05
BF	6	VAL	-	INSERTION	UNP Q72I05
DF	2	LYS	-	INSERTION	UNP Q72I05
DF	3	GLU	-	INSERTION	UNP Q72I05
DF	4	VAL	-	INSERTION	UNP Q72I05
DF	5	ALA	-	INSERTION	UNP Q72I05
DF	6	VAL	-	INSERTION	UNP Q72I05

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
29	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	5	VAL	LEU	CONFLICT	UNP Q72I16
DG	5	VAL	LEU	CONFLICT	UNP Q72I16

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			
30	DH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BJ	170	Total	C	N	O	0	0	0
			851	510	170	171			
31	DJ	170	Total	C	N	O	0	0	0
			851	510	170	171			

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	140	Total 1035	C 659	N 183	O 188	S 5	0	0	0
32	DK	140	Total 1035	C 659	N 183	O 188	S 5	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BO	122	Total 933	C 588	N 171	O 170	S 4	0	0	0
33	DO	122	Total 933	C 588	N 171	O 170	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	69	ILE	VAL	CONFLICT	UNP Q72I14
DO	69	ILE	VAL	CONFLICT	UNP Q72I14

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BP	146	Total 1114	C 692	N 227	O 193	S 2	0	0	0
34	DP	146	Total 1114	C 692	N 227	O 193	S 2	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BQ	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0
35	DQ	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	CONFLICT	UNP Q72I11
DQ	32	TYR	PHE	CONFLICT	UNP Q72I11

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BR	117	Total 960	C 599	N 202	O 159	0	0	0
36	DR	117	Total 960	C 599	N 202	O 159	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BS	99	Total 775	C 488	N 155	O 132	0	0	0
37	DS	99	Total 775	C 488	N 155	O 132	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BT	138	Total 1147	C 713	N 235	O 198	S 1	0	0	0
38	DT	138	Total 1147	C 713	N 235	O 198	S 1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	123	GLN	LYS	CONFLICT	UNP Q72JU9
BT	135	ALA	VAL	CONFLICT	UNP Q72JU9
DT	123	GLN	LYS	CONFLICT	UNP Q72JU9
DT	135	ALA	VAL	CONFLICT	UNP Q72JU9

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0
39	DU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0
41	DW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BX	93	Total 734	C 477	N 132	O 125	0	0	0
42	DX	93	Total 734	C 477	N 132	O 125	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BY	107	Total 818	C 524	N 155	O 134	S 5	0	0	0
43	DY	107	Total 818	C 524	N 155	O 134	S 5	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BZ	185	Total 1473	C 939	N 262	O 270	S 2	0	0	0
44	DZ	185	Total 1473	C 939	N 262	O 270	S 2	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B0	84	Total 662	C 410	N 140	O 111	S 1	0	0	0
45	D0	84	Total 662	C 410	N 140	O 111	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	11	ARG	LYS	CONFLICT	UNP Q72HR3
D0	11	ARG	LYS	CONFLICT	UNP Q72HR3

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
46	D1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	LYS	ARG	CONFLICT	UNP Q72G84
D1	81	LYS	ARG	CONFLICT	UNP Q72G84

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			
47	D4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			

- Molecule 48 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
48	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	60	Total 477	C 303	N 91	O 82	S 1	0	0	0
50	D3	60	Total 477	C 303	N 91	O 82	S 1	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total 459	C 288	N 90	O 76	S 5	0	0	0
51	D5	59	Total 459	C 288	N 90	O 76	S 5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	29	THR	ILE	CONFLICT	UNP P62652
D5	29	THR	ILE	CONFLICT	UNP P62652

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	50	Total 433	C 270	N 88	O 71	S 4	0	0	0
52	D6	50	Total 433	C 270	N 88	O 71	S 4	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	49	Total 430	C 263	N 108	O 57	S 2	0	0	0
53	D7	49	Total 430	C 263	N 108	O 57	S 2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total 517	C 331	N 102	O 82	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	Be	102	Total	C	N	O	0	0	0
			686	430	119	137			
56	De	102	Total	C	N	O	0	0	0
			686	430	119	137			

- Molecule 57 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	Bf	31	Total	C	N	O	0	0	0
			156	93	31	32			
57	Bg	31	Total	C	N	O	0	0	0
			156	93	31	32			
57	Df	31	Total	C	N	O	0	0	0
			156	93	31	32			
57	Dg	31	Total	C	N	O	0	0	0
			156	93	31	32			

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	Bh	30	Total	C	N	O	0	0	0
			151	90	30	31			
58	Dh	30	Total	C	N	O	0	0	0
			151	90	30	31			

- Molecule 59 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0
59	DB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0

- Molecule 60 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BA	2879	Total 61997	C 27594	N 11582	O 19943	P 2878	0	0	0
60	DA	2879	Total 61997	C 27594	N 11582	O 19943	P 2878	0	0	0

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).
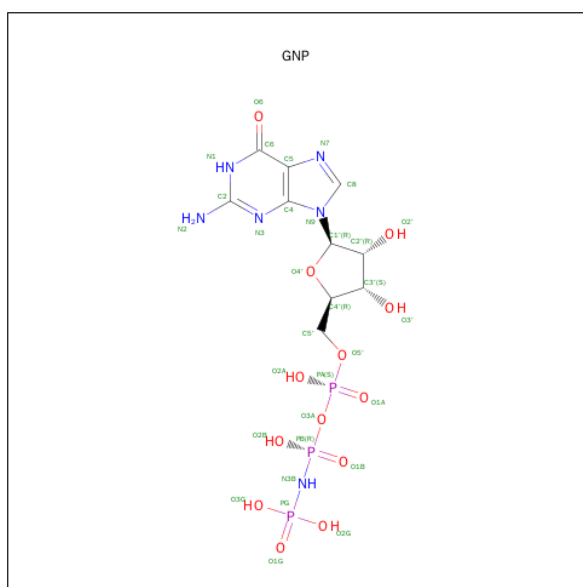
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total 32	C 10	N 6	O 13	P 3	0	0
61	CY	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total 1	Mg 1	0	0

MolProbity and EDS were not executed - this setion will therefore be empty.

3 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	302.39Å 683.92Å 356.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.86	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.86)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.34	Depositor
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.264 , 0.317	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	308202	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity was not executed - this section will therefore be empty.

4.2 Too-close contacts (i)

MolProbity was not executed - this section will therefore be empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity was not executed - this section will therefore be empty.

4.3.2 Protein sidechains (i)

MolProbity was not executed - this section will therefore be empty.

4.3.3 RNA (i)

MolProbity was not executed - this section will therefore be empty.

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

validation-pack and Mogul were not executed - this section will therefore be empty.

4.5 Carbohydrates (i)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.6 Ligand geometry (i)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.7 Other polymers (i)

validation-pack and Mogul were not executed - this section will therefore be empty.

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 was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

5.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

5.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

5.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.