Full wwPDB EM Validation Report (i)

Apr 16, 2024 – 07:59 am BST

PDB ID	:	5MDW
EMDB ID	:	EMD-3490
Title	:	Structure of ArfA(A18T) and RF2 bound to the 70S ribosome (pre-accommodated state)
Authors	:	James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on	:	2016-11-13
Resolution	:	3.06 Å(reported)

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 (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:

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.06 Å.

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

MolProbity failed to run properly - 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 149607 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	887	A	U	conflict	GB 802133627

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	120	2569	1144	468	837	120	0	0

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	5	109	49	22	33	5	0	0

- Molecule 5 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	5	76	1622	725	292	528	76	1	0	0

- Molecule 6 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	32	261	164	53	43	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	0	HIS	-	expression tag	UNP P36675
6	18	THR	ALA	engineered mutation	UNP P36675

- Molecule 7 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	341	2706	1669	470	558	9	0	0

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B	271	2082	1288	423	364	7	0	0

- Molecule 9 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	209	1565	979	288	294	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	201	1552	974	283	290	5	0	0

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	177	1410	899	249	256	6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	175	1313	826	241	244	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	149	1111	699	197	214	1	0	0

- Molecule 14 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	H	130	980	620	174	182	4	0	0

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	I	135	984	622	171	185	6	0	0

- Molecule 16 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	J	142	1129	714	212	199	4	0	0

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	K	123	946	593	181	166	6	0	0

- Molecule 18 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	L	144	1053	654	207	190	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	M	136	1074	686	205	177	6	0	0

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	119	951	588	195	163	5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	O	116	892	552	178	162	0	0

- Molecule 22 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	P	114	917	574	179	163	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	Q	117	947	604	192	151	0	0

- Molecule 24 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	R	103	816	516	153	145	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	S	110	857	532	166	156	3	0	0

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	T	94	746	470	140	134	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	U	103	788	498	148	142	0	0

- Molecule 28 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	94	753	479	137	134	3	0	0

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	76	582	360	117	104	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	X	77	625	388	129	106	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Y	62	501	308	98	94	1	0	0

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Z	58	448	281	87	78	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	a	66	522	323	99	94	6	0	0

- Molecule 34 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	b	56	444	269	94	80	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	c	52	426	275	78	73	0	0

- Molecule 36 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	d	46	377	228	90	57	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	e	64	504	323	105	74	2	0	0

- Molecule 38 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	f	38	302	185	65	48	4	0	0

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	g	225	1760	1113	316	323	8	0	0

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	h	208	1636	1036	307	290	3	0	0

- Molecule 41 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	i	205	1643	1026	315	298	4	0	0

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	156	1152	717	217	212	6	0	0

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	k	104	848	536	153	152	7	0	0

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	l	151	1181	735	227	215	4	0	0

- Molecule 45 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	m	129	979	616	173	184	6	0	0

- Molecule 46 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	127	1022	634	206	179	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	99	790	495	151	143	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	p	117	877	540	174	160	3	0	0

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	q	123	957	591	196	165	5	0	0

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	r	116	900	558	181	158	3	0	0

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	s	100	805	499	164	139	3	0	0

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	t	88	714	439	144	130	1	0	0

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	u	82	649	406	128	114	1	0	0

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	v	80	648	411	121	113	3	0	0

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	w	66	544	344	102	97	1	0	0

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	x	83	663	424	126	111	2	0	0

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	y	86	669	414	138	114	3	0	0

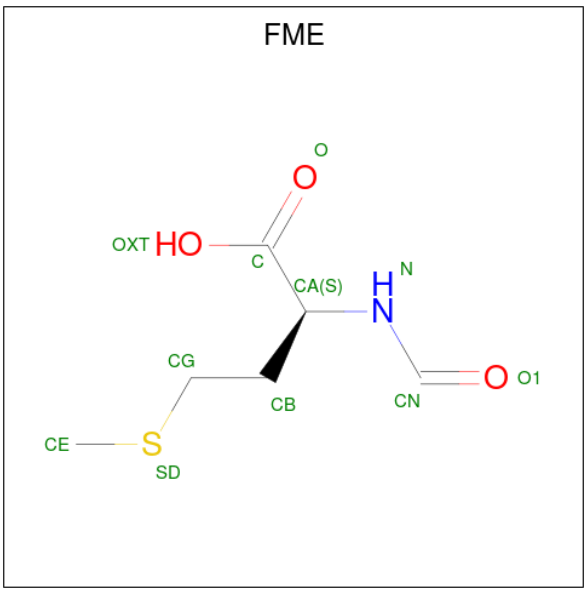
- Molecule 58 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	z	70	589	366	125	97	1	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
59	1	295	295	295	0
59	2	133	133	133	0
59	3	6	6	6	0
59	5	2	2	2	0
59	b	1	1	1	0
59	i	1	1	1	0

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	5	1	10	6	1	2	1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
61	a	1	1	1	0
61	f	1	1	1	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
62	B	2	2	2	0

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

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141950	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134615	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	2MG	2	1516	2	18,26,27	1.26	3 (16%)	16,38,41	1.59	3 (18%)
1	6MZ	1	1618	1	18,25,26	0.95	1 (5%)	16,36,39	1.65	2 (12%)
5	H2U	5	20	5	18,21,22	0.63	0	21,30,33	1.93	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	2MG	1	1835	1	18,26,27	1.21	3 (16%)	16,38,41	1.61	3 (18%)
49	0TD	q	89	49	7,9,10	6.74	5 (71%)	6,11,13	4.11	2 (33%)
2	2MG	2	1207	2	18,26,27	1.63	4 (22%)	16,38,41	1.07	1 (6%)
5	8AN	5	76	60,59,1,5	19,24,25	0.68	0	13,35,38	0.83	1 (7%)
2	UR3	2	1498	2	19,22,23	1.35	2 (10%)	26,32,35	1.24	5 (19%)
1	OMG	1	2251	1,5	18,26,27	1.67	4 (22%)	19,38,41	2.15	5 (26%)
1	PSU	1	2457	1	18,21,22	2.15	1 (5%)	22,30,33	1.54	4 (18%)
2	7MG	2	527	59,2	22,26,27	1.47	4 (18%)	29,39,42	2.86	12 (41%)
1	5MU	1	747	1	19,22,23	0.75	1 (5%)	28,32,35	1.01	3 (10%)
2	PSU	2	516	59,2	18,21,22	1.57	1 (5%)	22,30,33	1.61	2 (9%)
1	PSU	1	955	1	18,21,22	2.17	2 (11%)	22,30,33	1.57	3 (13%)
1	5MU	1	1939	59,1	19,22,23	0.84	1 (5%)	28,32,35	0.99	3 (10%)
1	OMU	1	2552	1	19,22,23	0.48	0	26,31,34	0.82	1 (3%)
5	PSU	5	55	5	18,21,22	1.86	1 (5%)	22,30,33	1.57	3 (13%)
1	2MA	1	2503	59,1	17,25,26	1.17	3 (17%)	17,37,40	3.14	6 (35%)
2	2MG	2	966	2	18,26,27	1.21	3 (16%)	16,38,41	2.15	3 (18%)
1	5MC	1	1962	1	18,22,23	0.85	1 (5%)	26,32,35	1.52	4 (15%)
1	PSU	1	2580	1	18,21,22	1.83	1 (5%)	22,30,33	1.61	3 (13%)
2	MA6	2	1518	2	18,26,27	0.58	0	19,38,41	0.76	0
1	PSU	1	1917	1	18,21,22	0.91	1 (5%)	22,30,33	1.01	1 (4%)
1	PSU	1	1911	1	18,21,22	1.44	4 (22%)	22,30,33	2.08	4 (18%)
1	PSU	1	2504	1	18,21,22	1.64	1 (5%)	22,30,33	1.65	3 (13%)
1	G7M	1	2069	1	20,26,27	1.64	1 (5%)	17,39,42	2.53	5 (29%)
5	5MU	5	54	5	19,22,23	0.64	0	28,32,35	1.00	3 (10%)
2	5MC	2	967	2	18,22,23	0.85	1 (5%)	26,32,35	1.45	3 (11%)
1	1MG	1	745	1	18,26,27	1.62	2 (11%)	19,39,42	2.04	4 (21%)
2	MA6	2	1519	2	18,26,27	0.59	0	19,38,41	0.83	1 (5%)
1	PSU	1	2605	1	18,21,22	1.98	1 (5%)	22,30,33	1.70	3 (13%)
5	4OC	5	32	5	20,23,24	0.59	0	26,32,35	1.21	2 (7%)
2	4OC	2	1402	2	20,23,24	1.18	2 (10%)	26,32,35	1.12	2 (7%)
2	5MC	2	1407	2	18,22,23	0.90	1 (5%)	26,32,35	1.30	3 (11%)
1	OMC	1	2498	59,1	19,22,23	1.14	2 (10%)	26,31,34	1.63	4 (15%)
1	3TD	1	1915	1	18,22,23	2.35	2 (11%)	22,32,35	2.63	6 (27%)
1	2MG	1	2445	1	18,26,27	1.24	2 (11%)	16,38,41	1.64	3 (18%)
5	4SU	5	8	5	18,21,22	1.64	3 (16%)	26,30,33	2.75	9 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	6MZ	1	1618	1	-	4/5/27/28	0/3/3/3
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
1	2MG	1	1835	1	-	0/5/27/28	0/3/3/3
49	0TD	q	89	49	-	2/7/12/14	-
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
5	8AN	5	76	60,59,1,5	-	3/3/25/26	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	OMG	1	2251	1,5	-	0/5/27/28	0/3/3/3
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
2	7MG	2	527	59,2	-	0/7/37/38	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	PSU	2	516	59,2	-	2/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	59,1	-	0/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
5	PSU	5	55	5	-	3/7/25/26	0/2/2/2
1	2MA	1	2503	59,1	-	1/3/25/26	0/3/3/3
2	2MG	2	966	2	-	3/5/27/28	0/3/3/3
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	1/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	1/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	2/3/25/26	0/3/3/3
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	5/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	MA6	2	1519	2	-	6/7/29/30	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	59,1	-	2/9/27/28	0/2/2/2
1	3TD	1	1915	1	-	5/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
5	4SU	5	8	5	-	2/7/25/26	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	q	89	0TD	CB-SB	-16.93	1.65	1.82
1	1	1915	3TD	C1'-C5	-9.08	1.29	1.50
1	1	955	PSU	C2'-C1'	-8.65	1.42	1.53
1	1	2457	PSU	C2'-C1'	-8.61	1.42	1.53
1	1	2605	PSU	C2'-C1'	-7.97	1.43	1.53
5	5	55	PSU	C2'-C1'	-7.67	1.43	1.53
1	1	2580	PSU	C2'-C1'	-7.43	1.44	1.53
1	1	2504	PSU	C2'-C1'	-6.55	1.45	1.53
2	2	516	PSU	C2'-C1'	-6.32	1.45	1.53
1	1	2069	G7M	C2'-C1'	-6.30	1.44	1.53
5	5	8	4SU	C4-S4	-4.73	1.59	1.68
1	1	745	1MG	C2'-C1'	-4.69	1.46	1.53
1	1	2251	OMG	C3'-C2'	-4.42	1.43	1.52
2	2	1207	2MG	C2'-C1'	-3.61	1.48	1.53
2	2	527	7MG	C4-N9	-3.52	1.33	1.37
1	1	2498	OMC	C3'-C2'	-3.48	1.45	1.52
49	q	89	0TD	CA-N	-3.17	1.37	1.47
2	2	1207	2MG	C6-N1	3.17	1.42	1.37
1	1	2445	2MG	C5-C6	-3.15	1.41	1.47
5	5	8	4SU	C5-C4	-2.97	1.38	1.42
1	1	1911	PSU	C4-N3	-2.95	1.33	1.38
2	2	1516	2MG	C5-C6	-2.95	1.41	1.47
1	1	745	1MG	C5-C6	-2.90	1.38	1.47
1	1	1835	2MG	C5-C6	-2.89	1.41	1.47
2	2	527	7MG	C5-N7	-2.88	1.32	1.35
2	2	527	7MG	C6-N1	-2.87	1.33	1.38
1	1	1962	5MC	C2'-C1'	-2.76	1.44	1.53
1	1	1939	5MU	C2'-C1'	-2.76	1.44	1.53
1	1	2251	OMG	C6-N1	2.75	1.42	1.37
2	2	966	2MG	C5-C6	-2.73	1.41	1.47
49	q	89	0TD	OD2-CG	-2.70	1.21	1.30
49	q	89	0TD	CB-CG	-2.68	1.47	1.52
1	1	2498	OMC	C2'-C1'	-2.66	1.46	1.53
2	2	966	2MG	C6-N1	2.65	1.41	1.37
1	1	1618	6MZ	C2'-C1'	-2.64	1.49	1.53
2	2	527	7MG	C5-C4	2.61	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1498	UR3	O4-C4	-2.57	1.18	1.23
49	q	89	0TD	CSB-SB	-2.53	1.74	1.79
2	2	1516	2MG	C6-N1	2.51	1.41	1.37
1	1	1911	PSU	C6-C5	2.50	1.38	1.35
2	2	967	5MC	C2'-C1'	-2.48	1.45	1.53
2	2	1207	2MG	C5-C4	-2.48	1.36	1.43
1	1	2445	2MG	C5-C4	-2.45	1.36	1.43
1	1	1915	3TD	C4-N3	-2.43	1.35	1.40
2	2	1407	5MC	C2'-C1'	-2.39	1.45	1.53
1	1	2503	2MA	C2'-C3'	-2.38	1.46	1.53
1	1	1835	2MG	C5-C4	-2.36	1.37	1.43
1	1	2251	OMG	C5-C6	-2.32	1.42	1.47
2	2	1402	4OC	C6-N1	-2.30	1.32	1.38
2	2	966	2MG	C5-C4	-2.27	1.37	1.43
1	1	1917	PSU	C2'-C1'	-2.22	1.50	1.53
1	1	955	PSU	C3'-C2'	-2.22	1.47	1.53
2	2	1516	2MG	C5-C4	-2.21	1.37	1.43
1	1	2251	OMG	C5-C4	-2.20	1.37	1.43
1	1	1835	2MG	C6-N1	2.18	1.41	1.37
1	1	1911	PSU	C2-N3	-2.16	1.33	1.37
1	1	747	5MU	C2'-C1'	-2.14	1.46	1.53
1	1	1911	PSU	C2-N1	-2.13	1.33	1.36
2	2	1498	UR3	C6-N1	-2.13	1.32	1.38
2	2	1207	2MG	C5-C6	-2.10	1.43	1.47
1	1	2503	2MA	C5-C4	-2.09	1.37	1.43
1	1	2503	2MA	C8-N7	-2.07	1.31	1.35
5	5	8	4SU	C4-N3	-2.05	1.35	1.37
2	2	1402	4OC	C2-N3	-2.01	1.32	1.36

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	527	7MG	N9-C4-N3	8.97	138.88	125.47
1	1	2503	2MA	C3'-C2'-C1'	-8.82	87.69	100.98
1	1	1915	3TD	O5'-C5'-C4'	7.70	135.17	108.99
49	q	89	0TD	CB-CA-N	-7.52	93.08	109.10
5	5	8	4SU	C5-C4-N3	7.17	121.34	114.69
2	2	966	2MG	O3'-C3'-C4'	6.98	131.23	111.05
5	5	8	4SU	C4-N3-C2	-6.94	120.60	127.34
1	1	2069	G7M	O2'-C2'-C3'	6.63	133.26	111.82
1	1	1911	PSU	N1-C2-N3	6.31	122.28	115.13
49	q	89	0TD	CSB-SB-CB	6.19	113.63	102.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1915	3TD	N1-C2-N3	6.01	120.88	116.14
5	5	8	4SU	C5-C4-S4	-5.98	116.77	124.47
2	2	967	5MC	O3'-C3'-C4'	5.70	127.52	111.05
1	1	745	1MG	C3'-C2'-C1'	5.57	109.37	100.98
2	2	527	7MG	C5-C4-N3	-5.51	117.62	128.13
2	2	516	PSU	O2'-C2'-C3'	5.47	129.52	111.82
2	2	527	7MG	N9-C8-N7	-5.24	95.89	103.38
1	1	1962	5MC	O3'-C3'-C4'	5.21	126.12	111.05
1	1	2498	OMC	O2'-C2'-C1'	5.21	119.24	109.08
1	1	2251	OMG	C3'-C2'-C1'	5.20	112.66	102.89
1	1	1618	6MZ	O3'-C3'-C4'	5.14	125.90	111.05
1	1	2498	OMC	O3'-C3'-C2'	5.11	125.69	111.17
5	5	55	PSU	O2'-C2'-C3'	5.11	128.34	111.82
1	1	2069	G7M	C3'-C2'-C1'	-5.04	93.39	100.98
1	1	2580	PSU	O2'-C2'-C3'	4.98	127.93	111.82
1	1	2504	PSU	O2'-C2'-C3'	4.92	127.73	111.82
5	5	20	H2U	O2'-C2'-C3'	4.89	127.66	111.82
2	2	1407	5MC	O3'-C3'-C2'	4.80	127.34	111.82
1	1	2504	PSU	O2'-C2'-C1'	4.73	122.52	111.23
1	1	955	PSU	O2'-C2'-C3'	4.67	126.93	111.82
2	2	1516	2MG	O3'-C3'-C2'	4.64	126.85	111.82
1	1	2605	PSU	O2'-C2'-C3'	4.61	126.74	111.82
1	1	2605	PSU	O2'-C2'-C1'	4.59	122.19	111.23
5	5	20	H2U	O3'-C3'-C2'	4.54	126.50	111.82
1	1	2457	PSU	O2'-C2'-C3'	4.53	126.49	111.82
1	1	2503	2MA	O4'-C1'-C2'	4.51	113.52	106.93
1	1	2503	2MA	O2'-C2'-C1'	4.48	127.40	110.85
1	1	1911	PSU	C4-N3-C2	-4.38	120.03	126.34
1	1	2503	2MA	O3'-C3'-C4'	4.36	123.66	111.05
1	1	2445	2MG	O3'-C3'-C2'	4.33	125.82	111.82
5	5	32	4OC	O3'-C3'-C2'	4.31	123.40	111.17
1	1	2251	OMG	O3'-C3'-C4'	4.27	123.39	111.05
1	1	1915	3TD	C5'-C4'-C3'	-4.25	99.26	115.18
1	1	2503	2MA	O3'-C3'-C2'	4.20	125.40	111.82
2	2	527	7MG	C2-N3-C4	4.10	119.61	112.30
1	1	745	1MG	O3'-C3'-C4'	4.09	122.89	111.05
1	1	1835	2MG	O3'-C3'-C4'	4.05	122.76	111.05
5	5	20	H2U	O3'-C3'-C4'	4.05	122.76	111.05
1	1	745	1MG	O3'-C3'-C2'	4.03	124.85	111.82
5	5	55	PSU	O2'-C2'-C1'	4.01	120.80	111.23
1	1	1915	3TD	C4-N3-C2	-3.99	120.28	124.61
1	1	1911	PSU	O2-C2-N1	-3.96	118.43	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	955	PSU	O2'-C2'-C1'	3.85	120.40	111.23
1	1	2251	OMG	O3'-C3'-C2'	3.79	121.93	111.17
1	1	2069	G7M	O2'-C2'-C1'	3.77	124.78	110.85
1	1	2580	PSU	O2'-C2'-C1'	3.60	119.82	111.23
2	2	516	PSU	O2'-C2'-C1'	3.53	119.66	111.23
1	1	2457	PSU	O2'-C2'-C1'	3.45	119.46	111.23
2	2	527	7MG	O4'-C4'-C3'	-3.44	98.30	105.11
1	1	1835	2MG	O3'-C3'-C2'	3.41	122.86	111.82
1	1	2580	PSU	C3'-C2'-C1'	3.41	105.61	101.64
5	5	20	H2U	O2'-C2'-C1'	3.38	121.34	110.02
2	2	527	7MG	O3'-C3'-C2'	3.29	122.45	111.82
5	5	8	4SU	C1'-N1-C2	3.24	123.43	117.57
1	1	1917	PSU	C3'-C2'-C1'	3.19	105.35	101.64
5	5	8	4SU	N3-C2-N1	3.16	119.08	114.89
2	2	966	2MG	C2'-C3'-C4'	-3.14	96.54	102.64
1	1	1618	6MZ	C2-N1-C6	3.05	119.20	116.59
5	5	32	4OC	O3'-C3'-C4'	2.98	119.68	111.05
1	1	955	PSU	C2'-C3'-C4'	-2.98	96.85	102.64
2	2	1498	UR3	O4'-C1'-C2'	-2.97	100.17	106.64
2	2	1516	2MG	O3'-C3'-C4'	2.93	119.53	111.05
1	1	1962	5MC	O3'-C3'-C2'	2.92	121.27	111.82
1	1	2069	G7M	O3'-C3'-C2'	2.87	121.12	111.82
1	1	2251	OMG	O2'-C2'-C1'	2.84	114.72	109.09
1	1	2445	2MG	C3'-C2'-C1'	2.82	105.23	100.98
1	1	2605	PSU	C2'-C3'-C4'	-2.80	97.21	102.64
1	1	2445	2MG	O3'-C3'-C4'	2.78	119.09	111.05
2	2	527	7MG	O3'-C3'-C4'	2.78	119.09	111.05
1	1	2457	PSU	C2'-C3'-C4'	-2.77	97.27	102.64
1	1	745	1MG	O2'-C2'-C3'	2.72	120.63	111.82
1	1	2503	2MA	O2'-C2'-C3'	2.72	120.62	111.82
2	2	527	7MG	C5-C6-N1	2.68	115.72	110.99
1	1	1962	5MC	C2'-C1'-N1	2.66	120.76	113.22
1	1	2069	G7M	C2'-C3'-C4'	-2.65	97.50	102.64
5	5	54	5MU	C2'-C1'-N1	2.58	120.54	113.22
2	2	1402	4OC	O4'-C4'-C3'	-2.58	100.00	105.11
1	1	747	5MU	C2'-C1'-N1	2.58	120.52	113.22
1	1	1835	2MG	C3'-C2'-C1'	2.55	104.82	100.98
5	5	8	4SU	C4'-O4'-C1'	-2.54	103.86	109.47
1	1	2251	OMG	C5'-C4'-C3'	2.54	124.71	115.18
1	1	1939	5MU	C2'-C1'-N1	2.51	120.32	113.22
2	2	1498	UR3	O2-C2-N3	-2.44	117.90	121.34
2	2	527	7MG	C3'-C2'-C1'	-2.44	96.80	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2498	OMC	O3'-C3'-C4'	2.43	118.07	111.05
2	2	1402	4OC	O2-C2-N3	-2.41	118.42	122.33
5	5	55	PSU	C3'-C2'-C1'	2.40	104.43	101.64
1	1	2504	PSU	C2'-C3'-C4'	-2.40	97.98	102.64
2	2	527	7MG	O6-C6-C5	-2.37	121.73	127.54
1	1	1962	5MC	C3'-C2'-C1'	2.36	105.92	101.43
2	2	1519	MA6	C2'-C3'-C4'	-2.36	98.05	102.64
5	5	8	4SU	O4'-C1'-N1	2.35	113.74	108.36
5	5	8	4SU	O4'-C1'-C2'	-2.27	101.70	106.64
1	1	1939	5MU	C4-N3-C2	-2.26	124.43	127.35
2	2	1207	2MG	O2'-C2'-C1'	-2.26	102.52	110.85
1	1	1939	5MU	N3-C2-N1	2.26	117.88	114.89
1	1	2457	PSU	C3'-C2'-C1'	2.24	104.24	101.64
2	2	527	7MG	C5-C4-N9	-2.23	103.45	106.35
1	1	1915	3TD	O4'-C4'-C5'	-2.18	102.19	109.37
1	1	747	5MU	N3-C2-N1	2.17	117.77	114.89
2	2	1407	5MC	O3'-C3'-C4'	2.15	117.28	111.05
2	2	1498	UR3	C1'-N1-C2	2.15	120.62	116.99
1	1	1915	3TD	C3'-C2'-C1'	2.12	104.11	101.64
5	5	54	5MU	N3-C2-N1	2.11	117.70	114.89
1	1	2552	OMU	N3-C2-N1	2.11	117.69	114.89
2	2	1516	2MG	C3'-C2'-C1'	2.10	104.14	100.98
1	1	2498	OMC	C3'-C2'-C1'	2.10	106.84	102.89
2	2	967	5MC	O3'-C3'-C2'	2.10	118.61	111.82
2	2	1498	UR3	C4-N3-C2	-2.08	122.61	124.56
2	2	527	7MG	O4'-C1'-N9	2.08	112.13	109.30
5	5	8	4SU	C6-C5-C4	-2.07	118.16	119.95
2	2	966	2MG	C3'-C2'-C1'	2.05	104.06	100.98
2	2	967	5MC	C2'-C1'-N1	2.04	119.00	113.22
2	2	1498	UR3	O3'-C3'-C4'	-2.03	105.18	111.05
5	5	54	5MU	C4-N3-C2	-2.03	124.73	127.35
5	5	76	8AN	C5-C6-N6	2.02	123.42	120.35
2	2	1407	5MC	O4'-C1'-C2'	2.01	111.03	106.64
1	1	1911	PSU	C5-C6-N1	-2.01	119.10	122.11
1	1	747	5MU	C4-N3-C2	-2.00	124.76	127.35

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	N3-C2-N2-CM2
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C9
2	2	1519	MA6	C5-C6-N6-C10
49	q	89	0TD	SB-CB-CG-OD2
5	5	20	H2U	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C6
5	5	55	PSU	C3'-C4'-C5'-O5'
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C2
5	5	76	8AN	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	516	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
5	5	20	H2U	C3'-C4'-C5'-O5'
5	5	55	PSU	O4'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
5	5	76	8AN	C4'-C5'-O5'-P
5	5	76	8AN	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C5-C6-N6-C9
5	5	8	4SU	O4'-C1'-N1-C2
49	q	89	0TD	CG-CB-SB-CSB
5	5	8	4SU	O4'-C1'-N1-C6
1	1	2069	G7M	C4'-C5'-O5'-P
1	1	2498	OMC	O4'-C4'-C5'-O5'
1	1	1911	PSU	O4'-C4'-C5'-O5'
2	2	967	5MC	C4'-C5'-O5'-P
1	1	2498	OMC	C3'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C6
1	1	1915	3TD	C4'-C5'-O5'-P
1	1	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	967	5MC	C2'-C1'-N1-C2
2	2	1519	MA6	C4'-C5'-O5'-P
5	5	55	PSU	C4'-C5'-O5'-P
1	1	2504	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 441 ligands modelled in this entry, 440 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	FME	5	101	5	8,9,10	0.54	0	7,9,11	1.22	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	FME	5	101	5	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	5	101	FME	O-C-CA	-3.16	116.50	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	5	101	FME	O1-CN-N-CA

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	2196:C	O3'	2197:U	P	2.55

5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3490. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections (i)

This section was not generated.

5.2 Central slices (i)

This section was not generated.

5.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

5.5 Orthogonal surface views (i)

This section was not generated.

5.6 Mask visualisation (i)

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

6 Map analysis (i)

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

6.1 Map-value distribution (i)

This section was not generated.

6.2 Volume estimate versus contour level (i)

This section was not generated.

6.3 Rotationally averaged power spectrum (i)

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

7 Fourier-Shell correlation (i)

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

8 Map-model fit (i)

This section was not generated.