

# wwPDB EM Validation Summary Report (i)

#### Apr 16, 2024 – 02:47 pm BST

PDB ID	:	6XZB
EMDB ID	:	EMD-10657
Title	:	E. coli 70S ribosome in complex with dirithromycin, fMet-Phe-tRNA(Phe) and
		deacylated tRNA(iMet) (focused classification).
Authors	:	Pichkur, E.B.; Polikanov, Y.S.; Myasnikov, A.G.; Konevega, A.L.
Deposited on	:	2020-02-03
Resolution	:	2.54  Å(reported)
Based on initial model	:	4YBB

This is a wwPDB EM Validation Summary 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{MapQ}$	:	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 2.54 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 55 unique types of molecules in this entry. The entry contains 145650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues		1	AltConf	Trace			
1	A1	1523	Total 32681	C 14576	N 5998	O 10584	Р 1523	0	0

• Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues		At		AltConf	Trace		
2	B1	224	Total 1753	C 1109	N 315	0 321	S 8	0	0

• Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues		At		AltConf	Trace		
3	C1	206	Total 1625	C 1028	N 305	O 289	${ m S} { m 3}$	0	0

• Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues		At		AltConf	Trace		
4	D1	205	Total 1643	C 1026	N 315	O 298	${f S}$ $4$	0	0

• Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues		At	oms		AltConf	Trace	
5	E1	155	Total 1144	C 711	N 216	0 211	S 6	0	0

• Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues		At	oms		AltConf	Trace	
6	F1	106	Total 862	C 545	N 156	0 154	S 7	0	0



• Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	G1	151	Total 1182	C 735	N 227	O 216	${f S}$ $4$	0	0

• Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms		AltConf	Trace	
8	H1	129	Total 979	C 616	N 173	0 184	S 6	0	0

• Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues		At	oms		AltConf	Trace	
9	I1	127	Total 1022	С 634	N 206	0 179	${ m S} { m 3}$	0	0

• Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues		At	oms		AltConf	Trace	
10	J1	99	Total 796	C 498	N 152	0 145	S 1	0	0

• Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	K1	117	Total 877	C 540	N 174	0 160	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues		At	oms	AltConf	Trace		
12	L1	122	Total 947	C 586	N 195	0 162	${S \atop 4}$	0	0

• Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	M1	114	Total 884	C 546	N 178	0 157	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called 30S ribosomal protein S14.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	N1	100	Total 805	C 499	N 164	O 139	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	01	88	Total 714	C 439	N 144	O 130	S 1	0	0

• Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	P1	82	Total 649	C 406	N 128	0 114	S 1	0	0

• Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
17	Q1	80	Total 649	C 411	N 121	0 114	S 3	0	0

• Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
18	R1	55	Total 456	C 288	N 86	O 82	0	0

• Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	S1	79	Total 638	C 408	N 120	0 108	${S \over 2}$	0	0

• Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues		At	oms			AltConf	Trace
20	T1	86	Total 670	C 414	N 138	0 115	${ m S} { m 3}$	0	0

• Molecule 21 is a protein called 30S ribosomal protein S21.



Mol	Chain	Residues		Atc	$\mathbf{ms}$			AltConf	Trace
21	U1	56	Total 465	C 290	N 96	0 78	S 1	0	0

• Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues		-	Atoms			AltConf	Trace
22	A2	2897	Total 62252	C 27778	N 11454	O 20121	Р 2899	3	0

• Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
23	B2	120	Total 2569	C 1144	N 468	O 837	Р 120	0	0

• Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		At	AltConf	Trace			
24	C2	271	Total 2083	C 1288	N 423	O 365	S 7	0	0

• Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
25	D2	209	Total 1566	C 980	N 288	0 294	$\frac{S}{4}$	1	0

• Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	AltConf	Trace			
26	E2	201	Total 1552	C 974	N 283	O 290	${S \atop 5}$	0	0

• Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
27	F2	177	Total 1411	C 899	N 249	O 257	S 6	0	0

• Molecule 28 is a protein called 50S ribosomal protein L6.



Mol	Chain	Residues		At	oms			AltConf	Trace
28	G2	176	Total 1323	C 832	N 243	O 246	${ m S} { m 2}$	0	0

• Molecule 29 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	H2	135	Total 1023	C 649	N 179	0 192	${ m S} { m 3}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H2	85	VAL	SER	conflict	UNP P0A7J3
H2	86	THR	MET	conflict	UNP P0A7J3

• Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues		At	AltConf	Trace			
30	I2	134	Total 979	C 619	N 169	0 185	S 6	0	0

• Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	J2	142	Total 1129	С 714	N 212	0 199	S 4	0	0

• Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			AltConf	Trace
32	K2	123	Total 946	C 593	N 181	0 166	S 6	0	0

• Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	L2	144	Total 1053	C 654	N 207	O 190	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 34 is a protein called 50S ribosomal protein L16.



Mol	Chain	Residues		At	oms			AltConf	Trace
34	M2	136	Total 1075	C 686	N 205	O 178	S 6	1	0

• Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	AltConf	Trace			
35	N2	125	Total 993	C 613	N 202	0 173	${ m S}{ m 5}$	0	0

• Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	O2	117	Total 900	C 557	N 179	0 163	S 1	0	0

• Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	AltConf	Trace			
37	P2	114	Total 917	C 574	N 179	0 163	S 1	0	0

• Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
38	Q2	117	Total 947	C 604	N 192	0 151	0	0

• Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	R2	103	Total 816	C 516	N 153	0 145	${ m S} { m 2}$	0	0

• Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	S2	110	Total 857	C 532	N 166	0 156	${ m S} { m 3}$	0	0

• Molecule 41 is a protein called 50S ribosomal protein L23.



Mol	Chain	Residues		At	oms	AltConf	Trace		
41	Τ2	93	Total 739	C 466	N 139	0 132	${ m S} { m 2}$	0	0

• Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
42	U2	102	Total 780	C 492	N 146	0 142	0	0

• Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	AltConf	Trace			
43	V2	94	Total 753	$\begin{array}{c} \mathrm{C} \\ 479 \end{array}$	N 137	0 134	${ m S} { m 3}$	0	0

• Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
44	W2	76	Total 580	C 359	N 117	O 103	S 1	1	0

• Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
45	X2	77	Total 625	C 388	N 129	O 106	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
46	V9	62	Total	С	Ν	Ο	$\mathbf{S}$	0	0
40	1 2	02	501	308	98	94	1	0	0

• Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
47	Z2	58	Total 449	C 281	N 87	O 79	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	2	0

• Molecule 48 is a protein called 50S ribosomal protein L32.



Mol	Chain	Residues		Atc	$\mathbf{ms}$			AltConf	Trace
48	a2	56	Total 444	C 269	N 94	O 80	S 1	0	0

• Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
49	b2	51	Total 414	C 266	N 76	O 72	0	0

• Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
50	c2	46	Total 377	C 228	N 90	O 57	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	d2	64	Total 504	C 323	N 105	0 74	${ m S} 2$	0	0

• Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
52	e2	38	Total 302	C 185	N 65	0 48	S 4	0	0

• Molecule 53 is a RNA chain called Deacylated tRNAi(Met).

Mol	Chain	Residues		-	AltConf	Trace				
53	f2	76	Total 1625	C 725	N 294	O 529	Р 76	S 1	0	0

• Molecule 54 is a RNA chain called fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
54	g2	76	Total 1667	C 760	N 297	0 534	Р 75	S 1	0	0

• Molecule 55 is Dirithromyc<br/>in (three-letter code: DI0) (formula:  $\rm C_{42}H_{78}N_2O_{14}).$ 





Mol	Chain	Residues	A	AltConf			
55	A2	1	Total 58	C 42	N 2	O 14	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	117919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	80	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	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)

45 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 Chai			Dec	es Link	B	ond leng	$\operatorname{gths}$	Bond angles			
MOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
53	4SU	f2	8	53	18,21,22	2.17	5 (27%)	26,30,33	1.70	6 (23%)	
54	5MC	g2	40	54	18,22,23	1.27	1 (5%)	26,32,35	2.12	10 (38%)	
22	2MG	A2	2445	22	18,26,27	<mark>3.39</mark>	7 (38%)	16,38,41	1.30	3 (18%)	



Mal	<b>T</b>	Chain	Dee	T : 1-	В	ond leng	gths	B	ond ang	gles
IVI01	Type	Chain	Res	Link	Counts	RMSZ	$\boxed{\# Z >2}$	Counts	RMSZ	# Z  > 2
22	5MC	A2	1962	22	18,22,23	2.01	6 (33%)	$26,\!32,\!35$	1.16	2 (7%)
22	1MG	A2	745	22	$18,\!26,\!27$	2.80	4 (22%)	$19,\!39,\!42$	1.28	3 (15%)
22	OMC	A2	2498	22	19,22,23	1.90	6 (31%)	26,31,34	0.96	1 (3%)
22	PSU	A2	2457	22	18,21,22	2.46	8 (44%)	22,30,33	1.90	4 (18%)
22	PSU	A2	2604	22	18,21,22	2.40	8 (44%)	22,30,33	1.87	4 (18%)
22	6MZ	A2	2030	22	18,25,26	1.98	1 (5%)	16,36,39	2.59	4 (25%)
22	OMG	A2	2251	53,22	18,26,27	2.46	5 (27%)	19,38,41	1.15	3 (15%)
54	2MG	g2	10	54	18,26,27	1.53	3 (16%)	16,38,41	1.64	4 (25%)
22	OMU	A2	2552	22	19,22,23	2.68	7 (36%)	26,31,34	1.86	6 (23%)
22	G7M	A2	2069	22	20,26,27	2.24	5 (25%)	17,39,42	0.71	0
54	M2G	g2	26	54	20,27,28	1.57	3 (15%)	22,40,43	1.06	2 (9%)
54	1MA	g2	58	54	16,25,26	1.62	3 (18%)	18,37,40	1.87	5 (27%)
53	PSU	f2	55	53	18,21,22	1.31	2 (11%)	22,30,33	1.91	4 (18%)
22	PSU	A2	1917	22	18,21,22	2.32	8 (44%)	22,30,33	1.82	4 (18%)
53	5MU	f2	54	53	19,22,23	1.44	5 (26%)	28,32,35	1.92	5 (17%)
54	5MC	g2	49	54	18,22,23	1.05	1 (5%)	26,32,35	1.59	4 (15%)
22	3TD	A2	1915	22	18,22,23	2.73	7 (38%)	22,32,35	1.89	2 (9%)
54	OMC	g2	32	54	19,22,23	1.39	3 (15%)	26,31,34	2.13	2 (7%)
22	PSU	A2	1911	22	18,21,22	2.32	8 (44%)	22,30,33	1.84	4 (18%)
54	5MU	g2	54	54	19,22,23	1.54	3 (15%)	28,32,35	2.42	7 (25%)
22	PSU	A2	2580	22	18,21,22	2.47	10 (55%)	22,30,33	1.90	<mark>5 (22%)</mark>
53	5MC	f2	32	53	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)
22	6MZ	A2	1618	22	18,25,26	1.98	1 (5%)	16,36,39	2.19	4 (25%)
22	PSU	A2	2504	22	18,21,22	2.39	8 (44%)	22,30,33	1.89	4 (18%)
54	PSU	g2	39	54	18,21,22	1.84	5 (27%)	22,30,33	2.49	7 (31%)
54	YYG	g2	37	54	31,42,43	2.16	7 (22%)	33,62,65	2.03	10 (30%)
54	7MG	g2	46	54	22,26,27	2.13	4 (18%)	29,39,42	3.15	10 (34%)
54	H2U	g2	17	54	18,21,22	1.00	2 (11%)	21,30,33	1.92	2 (9%)
54	31M	g2	76	22	38,44,45	4.34	18 (47%)	38,61,64	2.23	13 (34%)
22	PSU	A2	955	22	18,21,22	2.44	8 (44%)	22,30,33	1.85	4 (18%)
22	PSU	A2	746	22	18,21,22	2.37	9(50%)	22,30,33	1.80	4 (18%)
22	5MU	A2	1939	22	19,22,23	2.67	7 (36%)	28,32,35	3.95	10 (35%)
54	PSU	g2	55	54	18,21,22	1.65	4 (22%)	22,30,33	2.11	4 (18%)
22	H2U	A2	2449	22	18,21,22	4.07	5 (27%)	21,30,33	5.20	7 (33%)
22	2MG	A2	1835	22	18,26,27	3.37	7 (38%)	16,38,41	1.35	3 (18%)



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	Bond angles		
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
22	PSU	A2	2605	22	18,21,22	2.39	8 (44%)	22,30,33	1.87	4 (18%)
54	OMG	g2	34	54	$18,\!26,\!27$	1.57	3 (16%)	19,38,41	1.52	4 (21%)
22	2MA	A2	2503	22	$17,\!25,\!26$	1.59	3 (17%)	17,37,40	1.04	2 (11%)
34	4D4	M2	81	34	9,11,12	2.03	2 (22%)	8,13,15	2.10	4 (50%)
25	MEQ	D2	150[A]	25	8,9,10	0.95	0	5,10,12	0.66	0
22	5MU	A2	747	$\overline{22}$	19,22,23	2.58	7 (36%)	28,32,35	3.81	11 (39%)
54	H2U	g2	16	54	18,21,22	0.99	2 (11%)	21,30,33	1.90	2 (9%)

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
53	4SU	f2	8	53	-	0/7/25/26	0/2/2/2
54	5MC	g2	40	54	-	0/7/25/26	0/2/2/2
22	2MG	A2	2445	22	-	2/5/27/28	0/3/3/3
22	5MC	A2	1962	22	-	2/7/25/26	0/2/2/2
22	1MG	A2	745	22	-	0/3/25/26	0/3/3/3
22	OMC	A2	2498	22	-	0/9/27/28	0/2/2/2
22	PSU	A2	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	2604	22	_	0/7/25/26	0/2/2/2
22	6MZ	A2	2030	22	-	2/5/27/28	0/3/3/3
22	OMG	A2	2251	53,22	-	1/5/27/28	0/3/3/3
54	2MG	g2	10	54	-	0/5/27/28	0/3/3/3
22	OMU	A2	2552	22	-	0/9/27/28	0/2/2/2
22	G7M	A2	2069	22	-	1/3/25/26	0/3/3/3
54	M2G	g2	26	54	-	0/7/29/30	0/3/3/3
54	1MA	g2	58	54	-	2/3/25/26	0/3/3/3
53	PSU	f2	55	53	-	0/7/25/26	0/2/2/2
22	PSU	A2	1917	22	-	0/7/25/26	0/2/2/2
53	$5 \mathrm{MU}$	f2	54	53	-	0/7/25/26	0/2/2/2
54	$5 \mathrm{MC}$	g2	49	54	-	3/7/25/26	0/2/2/2
22	3TD	A2	1915	22	-	0/7/25/26	0/2/2/2
54	OMC	g2	32	54	-	0/9/27/28	0/2/2/2
22	PSU	A2	1911	22	_	0/7/25/26	0/2/2/2
54	$5 \mathrm{MU}$	g2	54	54	-	2/7/25/26	0/2/2/2
22	PSU	A2	2580	22	-	0/7/25/26	0/2/2/2
53	5MC	f2	32	53	-	0/7/25/26	0/2/2/2
22	6MZ	A2	1618	22	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	A2	2504	22	-	2/7/25/26	0/2/2/2
54	PSU	g2	39	54	-	3/7/25/26	0/2/2/2
54	YYG	g2	37	54	-	16/20/42/43	0/3/4/4
54	7MG	g2	46	54	-	3/7/37/38	0/3/3/3
54	H2U	g2	17	54	-	5/7/38/39	0/2/2/2
54	31M	g2	76	22	-	6/27/49/50	0/4/4/4
22	PSU	A2	955	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	746	22	-	2/7/25/26	0/2/2/2
22	5MU	A2	1939	22	-	0/7/25/26	0/2/2/2
54	PSU	g2	55	54	-	0/7/25/26	0/2/2/2
22	H2U	A2	2449	22	-	0/7/38/39	0/2/2/2
22	2MG	A2	1835	22	-	0/5/27/28	0/3/3/3
22	PSU	A2	2605	22	-	0/7/25/26	0/2/2/2
54	OMG	g2	34	54	-	3/5/27/28	0/3/3/3
22	2MA	A2	2503	22	-	1/3/25/26	0/3/3/3
34	4D4	M2	81	34	-	3/11/12/14	-
25	MEQ	D2	150[A]	25	-	4/8/9/11	-
22	5MU	A2	747	22	-	0/7/25/26	0/2/2/2
54	H2U	g2	16	54	-	3/7/38/39	0/2/2/2

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The worst 5 of 231 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	g2	76	31M	C2'-C1'	-16.92	1.28	1.53
54	g2	76	31M	O4'-C1'	12.06	1.57	1.41
22	A2	2449	H2U	O4-C4	10.10	1.43	1.23
54	g2	76	31M	O4'-C4'	-9.47	1.23	1.45
22	A2	1835	2MG	O6-C6	9.24	1.42	1.23

The worst 5 of 206 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
22	A2	2449	H2U	C4-N3-C2	-15.23	113.16	125.79
22	A2	2449	H2U	O2-C2-N1	-11.49	108.68	123.11
54	g2	46	7MG	N9-C4-N3	10.82	141.66	125.47
54	g2	32	OMC	C2'-C1'-N1	-9.28	96.21	114.22
22	A2	1939	5MU	C4-N3-C2	-9.13	115.53	127.35

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
25	D2	150[A]	MEQ	N-CA-CB-CG
34	M2	81	4D4	NE-CD-CG-CB
22	A2	746	PSU	C2'-C1'-C5-C4
22	A2	2251	OMG	C1'-C2'-O2'-CM2
54	g2	17	H2U	C3'-C4'-C5'-O5'

5 of 66 torsion outliers are listed below:

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)

1 ligand is 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).

Mal	Turne	Chain	Dec	Link Bond lengths			Bond angles			
MOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
55	DI0	A2	3001	-	$58,\!61,\!61$	1.62	11 (18%)	77,92,92	1.65	20 (25%)

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
55	DI0	A2	3001	-	-	10/70/121/121	0/3/4/4

The worst 5 of 11 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
55	A2	3001	DI0	CAF-CAE	-5.60	1.39	1.51
55	A2	3001	DI0	OBI-CAG	-4.12	1.33	1.43
55	A2	3001	DI0	OAU-CBG	-3.41	1.38	1.44
55	A2	3001	DI0	OAY-CAC	-3.13	1.35	1.43
55	A2	3001	DI0	CBC-CBB	2.86	1.58	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
55	A2	3001	DI0	OAL-CAW-CBT	4.88	116.70	107.40
55	A2	3001	DI0	CBT-CAW-CAD	-4.69	106.31	115.20
55	A2	3001	DI0	OBK-CAN-CAX	4.22	110.07	103.81
55	A2	3001	DI0	CAP-CAH-CAJ	-3.35	109.30	114.05
55	A2	3001	DI0	CBR-CAP-CBC	-2.75	106.45	111.09

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
55	A2	3001	DI0	NAQ-CBA-CBS-OBW
55	A2	3001	DI0	NAQ-CAK-CBB-CBC
55	A2	3001	DI0	CAJ-CAH-CAP-OBJ
55	A2	3001	DI0	OBX-CCC-CCD-OBW
55	A2	3001	DI0	OAL-CAW-CBT-CCF

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





#### 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
22	A2	1
54	g2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	885:C	O3'	892:A	Р	11.25
1	g2	75:C	O3'	76:31M	Р	1.09



## 5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10657. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 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.

