Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 07:56 am BST

PDB ID	:	6XZA
EMDB ID	:	EMD-10656
Title	:	E. coli 70S ribosome in complex with dirithromycin, 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	:	2.66 Å(reported)
Based on initial model	:	4YBB

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

EMDB validation analysis	:	0.0.1.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)
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 2.66 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 54 unique types of molecules in this entry. The entry contains 143983 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C1	206	1625	1028	305	289	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D1	205	1643	1026	315	298	4	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	122	Total	C	N	O	S	0	0
			947	586	195	162	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D2	209	Total	C	N	O	S	1	0
			1566	980	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E2	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G2	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H2	135	Total	C	N	O	S	0	0
			1023	649	179	192	3		

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	Atoms					AltConf	Trace
30	I2	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J2	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L2	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N2	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R2	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S2	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T2	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V2	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W2	76	Total	C	N	O	S	1	0
			580	359	117	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X2	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y2	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z2	58	Total	C	N	O	S	2	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	a2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	c2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	d2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

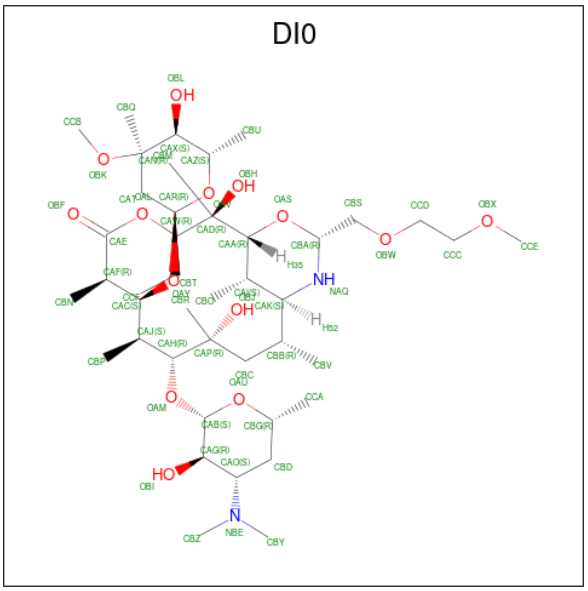
- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	e2	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

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

- Molecule 54 is Dirithromycin (three-letter code: DI0) (formula: $C_{42}H_{78}N_2O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
54	A2	1	Total	C	N	O	0
			58	42	2	14	

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	66269	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 ($e^-/Å^2$)	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

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

30 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	$\#\|Z\| > 2$
22	OMU	A2	2552	22	19,22,23	2.68	7 (36%)	26,31,34	1.86	6 (23%)
25	MEQ	D2	150[A]	25	8,9,10	0.95	0	5,10,12	0.66	0
22	PSU	A2	1917	22	18,21,22	2.32	8 (44%)	22,30,33	1.82	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	PSU	f2	55	53	18,21,22	2.37	5 (27%)	22,30,33	3.19	12 (54%)
53	5MC	f2	32	53	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)
22	PSU	A2	746	22	18,21,22	2.37	9 (50%)	22,30,33	1.80	4 (18%)
22	OMG	A2	2251	22,53	18,26,27	2.46	5 (27%)	19,38,41	1.15	3 (15%)
34	4D4	M2	81	34	9,11,12	2.03	2 (22%)	8,13,15	2.10	4 (50%)
22	2MG	A2	2445	22	18,26,27	3.39	7 (38%)	16,38,41	1.30	3 (18%)
53	4SU	f2	8	53	18,21,22	5.37	13 (72%)	26,30,33	5.68	15 (57%)
22	5MU	A2	747	22	19,22,23	2.58	7 (36%)	28,32,35	3.81	11 (39%)
22	H2U	A2	2449	22	18,21,22	4.07	5 (27%)	21,30,33	5.20	7 (33%)
53	5MU	f2	54	53	19,22,23	2.68	6 (31%)	28,32,35	3.28	14 (50%)
22	3TD	A2	1915	22	18,22,23	2.73	7 (38%)	22,32,35	1.89	2 (9%)
22	PSU	A2	955	22	18,21,22	2.44	8 (44%)	22,30,33	1.85	4 (18%)
22	PSU	A2	1911	22	18,21,22	2.32	8 (44%)	22,30,33	1.84	4 (18%)
22	2MA	A2	2503	22	17,25,26	1.59	3 (17%)	17,37,40	1.04	2 (11%)
22	PSU	A2	2605	22	18,21,22	2.39	8 (44%)	22,30,33	1.87	4 (18%)
22	5MC	A2	1962	22	18,22,23	2.01	6 (33%)	26,32,35	1.16	2 (7%)
22	6MZ	A2	1618	22	18,25,26	1.98	1 (5%)	16,36,39	2.19	4 (25%)
22	5MU	A2	1939	22	19,22,23	2.67	7 (36%)	28,32,35	3.95	10 (35%)
22	G7M	A2	2069	22	20,26,27	2.24	5 (25%)	17,39,42	0.71	0
22	PSU	A2	2580	22	18,21,22	2.47	10 (55%)	22,30,33	1.90	5 (22%)
22	2MG	A2	1835	22	18,26,27	3.37	7 (38%)	16,38,41	1.35	3 (18%)
22	1MG	A2	745	22	18,26,27	2.80	4 (22%)	19,39,42	1.28	3 (15%)
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	PSU	A2	2504	22	18,21,22	2.39	8 (44%)	22,30,33	1.89	4 (18%)
22	6MZ	A2	2030	22	18,25,26	1.98	1 (5%)	16,36,39	2.59	4 (25%)
22	OMC	A2	2498	22	19,22,23	1.90	6 (31%)	26,31,34	0.96	1 (3%)

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
22	OMU	A2	2552	22	-	0/9/27/28	0/2/2/2
25	MEQ	D2	150[A]	25	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	A2	1917	22	-	0/7/25/26	0/2/2/2
53	PSU	f2	55	53	-	5/7/25/26	0/2/2/2
53	5MC	f2	32	53	-	0/7/25/26	0/2/2/2
22	PSU	A2	746	22	-	2/7/25/26	0/2/2/2
22	OMG	A2	2251	22,53	-	1/5/27/28	0/3/3/3
34	4D4	M2	81	34	-	3/11/12/14	-
22	2MG	A2	2445	22	-	2/5/27/28	0/3/3/3
53	4SU	f2	8	53	-	0/7/25/26	0/2/2/2
22	5MU	A2	747	22	-	0/7/25/26	0/2/2/2
22	H2U	A2	2449	22	-	0/7/38/39	0/2/2/2
53	5MU	f2	54	53	-	0/7/25/26	0/2/2/2
22	3TD	A2	1915	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	955	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	1911	22	-	0/7/25/26	0/2/2/2
22	2MA	A2	2503	22	-	1/3/25/26	0/3/3/3
22	PSU	A2	2605	22	-	0/7/25/26	0/2/2/2
22	5MC	A2	1962	22	-	2/7/25/26	0/2/2/2
22	6MZ	A2	1618	22	-	0/5/27/28	0/3/3/3
22	5MU	A2	1939	22	-	0/7/25/26	0/2/2/2
22	G7M	A2	2069	22	-	1/3/25/26	0/3/3/3
22	PSU	A2	2580	22	-	0/7/25/26	0/2/2/2
22	2MG	A2	1835	22	-	0/5/27/28	0/3/3/3
22	1MG	A2	745	22	-	0/3/25/26	0/3/3/3
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	PSU	A2	2504	22	-	2/7/25/26	0/2/2/2
22	6MZ	A2	2030	22	-	2/5/27/28	0/3/3/3
22	OMC	A2	2498	22	-	0/9/27/28	0/2/2/2

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	f2	8	4SU	C4-S4	-14.35	1.41	1.68
53	f2	8	4SU	C4-N3	-10.75	1.26	1.37
22	A2	2449	H2U	O4-C4	10.10	1.43	1.23
22	A2	1835	2MG	O6-C6	9.24	1.42	1.23
22	A2	2445	2MG	O6-C6	9.16	1.41	1.23
22	A2	745	1MG	O6-C6	9.03	1.40	1.22
22	A2	1915	3TD	O4-C4	8.17	1.40	1.23
22	A2	2449	H2U	C2-N1	8.08	1.47	1.35
22	A2	2449	H2U	O2-C2	8.07	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	2552	OMU	O4-C4	7.89	1.39	1.24
22	A2	1618	6MZ	C6-N6	7.88	1.47	1.35
22	A2	2030	6MZ	C6-N6	7.75	1.47	1.35
53	f2	8	4SU	C5-C4	-7.67	1.32	1.42
22	A2	1939	5MU	C2-N1	-6.47	1.28	1.38
53	f2	8	4SU	C2-N3	-6.46	1.26	1.38
22	A2	2251	OMG	O6-C6	6.41	1.36	1.23
22	A2	2069	G7M	O6-C6	6.32	1.36	1.23
22	A2	2449	H2U	C2-N3	6.14	1.48	1.38
22	A2	747	5MU	C2-N1	-6.10	1.28	1.38
53	f2	54	5MU	C2-N3	-6.01	1.27	1.38
53	f2	55	PSU	C2-N1	-5.71	1.29	1.36
22	A2	1835	2MG	C2-N2	5.69	1.46	1.33
22	A2	2445	2MG	C2-N2	5.64	1.45	1.33
22	A2	1835	2MG	CM2-N2	5.35	1.55	1.45
53	f2	55	PSU	C2-N3	-5.30	1.28	1.37
53	f2	54	5MU	C6-N1	-5.30	1.29	1.38
22	A2	2445	2MG	CM2-N2	5.22	1.54	1.45
53	f2	54	5MU	C4-N3	-5.12	1.29	1.38
22	A2	745	1MG	C2-N2	5.06	1.43	1.34
22	A2	2251	OMG	C6-N1	-5.05	1.30	1.37
22	A2	2580	PSU	C1'-C5	-4.84	1.39	1.50
22	A2	2604	PSU	C1'-C5	-4.81	1.39	1.50
22	A2	2457	PSU	C1'-C5	-4.80	1.39	1.50
22	A2	2445	2MG	C6-N1	-4.80	1.30	1.37
22	A2	2069	G7M	C2-N2	4.76	1.45	1.34
34	M2	81	4D4	CZ-NE	4.74	1.42	1.33
22	A2	1939	5MU	C2-N3	-4.73	1.29	1.38
22	A2	2449	H2U	C4-N3	4.73	1.45	1.37
22	A2	1917	PSU	C1'-C5	-4.71	1.39	1.50
22	A2	955	PSU	C1'-C5	-4.70	1.39	1.50
22	A2	2605	PSU	C1'-C5	-4.69	1.39	1.50
22	A2	746	PSU	C1'-C5	-4.68	1.39	1.50
22	A2	2504	PSU	C1'-C5	-4.67	1.39	1.50
22	A2	1911	PSU	C1'-C5	-4.66	1.39	1.50
22	A2	2498	OMC	C4-N4	4.65	1.44	1.33
22	A2	1939	5MU	C6-N1	-4.62	1.30	1.38
22	A2	2503	2MA	C6-N6	4.61	1.47	1.28
22	A2	1835	2MG	C6-N1	-4.60	1.31	1.37
22	A2	747	5MU	C2-N3	-4.58	1.29	1.38
22	A2	2552	OMU	C2-N1	-4.55	1.31	1.38
22	A2	2251	OMG	C2-N2	4.53	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	747	5MU	C6-N1	-4.46	1.30	1.38
53	f2	8	4SU	O2-C2	-4.44	1.14	1.23
53	f2	8	4SU	C2'-C1'	-4.39	1.39	1.53
22	A2	1962	5MC	C4-N4	4.17	1.45	1.34
22	A2	2069	G7M	C6-N1	-4.16	1.31	1.37
22	A2	2457	PSU	C4-N3	-4.03	1.31	1.38
22	A2	2580	PSU	C4-N3	-4.03	1.31	1.38
22	A2	1962	5MC	C2-N1	-4.02	1.31	1.40
22	A2	955	PSU	C2-N1	-4.01	1.31	1.36
22	A2	1915	3TD	C2-N1	-3.99	1.31	1.37
22	A2	2457	PSU	C2-N1	-3.96	1.31	1.36
22	A2	955	PSU	C4-N3	-3.96	1.31	1.38
22	A2	2605	PSU	C4-N3	-3.93	1.31	1.38
22	A2	1915	3TD	C4-N3	-3.89	1.32	1.40
22	A2	2504	PSU	C4-N3	-3.89	1.31	1.38
22	A2	2580	PSU	C2-N1	-3.89	1.31	1.36
22	A2	2445	2MG	C5-C6	-3.89	1.39	1.47
22	A2	2604	PSU	C4-N3	-3.86	1.31	1.38
22	A2	2552	OMU	C4-N3	-3.83	1.31	1.38
22	A2	1962	5MC	C6-N1	-3.83	1.31	1.38
22	A2	2504	PSU	C2-N1	-3.82	1.31	1.36
22	A2	1835	2MG	C5-C6	-3.81	1.39	1.47
22	A2	2604	PSU	C2-N1	-3.80	1.31	1.36
22	A2	2605	PSU	C2-N1	-3.79	1.31	1.36
22	A2	746	PSU	C4-N3	-3.77	1.31	1.38
22	A2	2457	PSU	C2-N3	-3.75	1.31	1.37
22	A2	1911	PSU	C4-N3	-3.75	1.31	1.38
22	A2	745	1MG	C6-N1	-3.75	1.32	1.39
22	A2	2605	PSU	C2-N3	-3.74	1.31	1.37
22	A2	2552	OMU	C2-N3	-3.73	1.31	1.38
22	A2	2498	OMC	C2-N1	-3.72	1.31	1.40
22	A2	1917	PSU	C4-N3	-3.72	1.31	1.38
22	A2	746	PSU	C2-N1	-3.70	1.31	1.36
22	A2	955	PSU	C2-N3	-3.69	1.31	1.37
22	A2	2580	PSU	C2-N3	-3.66	1.31	1.37
22	A2	2604	PSU	C2-N3	-3.65	1.31	1.37
22	A2	1911	PSU	C2-N1	-3.64	1.31	1.36
22	A2	2504	PSU	C2-N3	-3.63	1.31	1.37
22	A2	1917	PSU	C2-N1	-3.63	1.31	1.36
22	A2	1939	5MU	C4-N3	-3.59	1.32	1.38
22	A2	746	PSU	C2-N3	-3.53	1.31	1.37
22	A2	747	5MU	C6-C5	3.52	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	1939	5MU	C6-C5	3.51	1.40	1.34
22	A2	1917	PSU	C2-N3	-3.48	1.31	1.37
53	f2	54	5MU	O4'-C4'	-3.47	1.37	1.45
22	A2	747	5MU	C4-N3	-3.47	1.32	1.38
22	A2	2445	2MG	C2-N1	-3.46	1.31	1.36
53	f2	8	4SU	O4'-C4'	-3.46	1.37	1.45
22	A2	1911	PSU	C2-N3	-3.42	1.31	1.37
22	A2	1835	2MG	C2-N1	-3.27	1.31	1.36
53	f2	55	PSU	O3'-C3'	3.20	1.50	1.43
22	A2	1915	3TD	C6-C5	3.10	1.38	1.35
22	A2	1915	3TD	C2-N3	-3.07	1.31	1.38
53	f2	8	4SU	C6-N1	-3.06	1.30	1.38
34	M2	81	4D4	CZ-NH2	3.03	1.44	1.32
22	A2	1962	5MC	O2-C2	-3.02	1.18	1.23
22	A2	1939	5MU	O4-C4	-3.00	1.17	1.23
22	A2	1939	5MU	O2-C2	-3.00	1.17	1.23
22	A2	2498	OMC	O2-C2	-2.99	1.18	1.23
22	A2	2605	PSU	O4-C4	-2.99	1.17	1.23
22	A2	2457	PSU	O4-C4	-2.98	1.17	1.23
22	A2	955	PSU	O4-C4	-2.97	1.17	1.23
22	A2	747	5MU	O4-C4	-2.97	1.17	1.23
22	A2	1911	PSU	C6-C5	2.95	1.38	1.35
22	A2	2580	PSU	O4-C4	-2.93	1.18	1.23
53	f2	54	5MU	C3'-C4'	-2.93	1.45	1.53
22	A2	1917	PSU	C6-C5	2.90	1.38	1.35
53	f2	8	4SU	C1'-N1	-2.90	1.39	1.47
22	A2	2504	PSU	C6-C5	2.90	1.38	1.35
22	A2	747	5MU	O2-C2	-2.89	1.17	1.23
22	A2	2604	PSU	O4-C4	-2.89	1.18	1.23
22	A2	746	PSU	C6-C5	2.89	1.38	1.35
22	A2	2504	PSU	O4-C4	-2.88	1.18	1.23
22	A2	746	PSU	O4-C4	-2.85	1.18	1.23
53	f2	55	PSU	C4-N3	-2.82	1.33	1.38
22	A2	2604	PSU	C6-C5	2.81	1.38	1.35
22	A2	2069	G7M	C2-N1	-2.78	1.30	1.37
22	A2	955	PSU	C6-C5	2.77	1.38	1.35
22	A2	1911	PSU	O4-C4	-2.75	1.18	1.23
22	A2	2580	PSU	C6-N1	-2.75	1.31	1.36
22	A2	2580	PSU	C6-C5	2.74	1.38	1.35
22	A2	2457	PSU	C6-C5	2.74	1.38	1.35
22	A2	2503	2MA	C6-N1	-2.73	1.31	1.38
22	A2	2552	OMU	O2-C2	-2.72	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	2605	PSU	C6-C5	2.72	1.38	1.35
22	A2	955	PSU	C6-N1	-2.72	1.31	1.36
53	f2	32	5MC	C6-N1	-2.70	1.33	1.38
22	A2	745	1MG	C5-C6	-2.69	1.39	1.47
22	A2	2457	PSU	C6-N1	-2.65	1.31	1.36
53	f2	8	4SU	C2-N1	-2.64	1.34	1.38
22	A2	1917	PSU	O4-C4	-2.64	1.18	1.23
53	f2	55	PSU	C6-N1	-2.64	1.31	1.36
53	f2	54	5MU	C4-C5	-2.63	1.40	1.44
22	A2	2605	PSU	C6-N1	-2.61	1.31	1.36
22	A2	2604	PSU	C6-N1	-2.60	1.31	1.36
22	A2	2457	PSU	O2-C2	-2.59	1.18	1.23
22	A2	2504	PSU	C6-N1	-2.59	1.31	1.36
22	A2	2580	PSU	O2-C2	-2.56	1.18	1.23
22	A2	2552	OMU	C6-N1	-2.55	1.31	1.38
22	A2	955	PSU	O2-C2	-2.55	1.18	1.23
22	A2	2251	OMG	C5-C6	-2.55	1.42	1.47
22	A2	1917	PSU	C6-N1	-2.54	1.32	1.36
22	A2	2498	OMC	C6-N1	-2.51	1.31	1.38
22	A2	1911	PSU	C6-N1	-2.49	1.32	1.36
22	A2	2605	PSU	O2-C2	-2.47	1.18	1.23
53	f2	8	4SU	O4'-C1'	-2.47	1.36	1.42
22	A2	1915	3TD	O2-C2	-2.45	1.18	1.23
22	A2	2504	PSU	O2-C2	-2.45	1.18	1.23
22	A2	1962	5MC	C2-N3	-2.44	1.31	1.36
22	A2	2604	PSU	O2-C2	-2.44	1.18	1.23
22	A2	2498	OMC	C2-N3	-2.42	1.31	1.36
22	A2	746	PSU	C6-N1	-2.41	1.32	1.36
22	A2	2552	OMU	C5-C4	-2.41	1.38	1.43
22	A2	1915	3TD	C6-N1	-2.39	1.32	1.36
22	A2	1917	PSU	O2-C2	-2.38	1.18	1.23
53	f2	32	5MC	C6-C5	2.35	1.38	1.34
22	A2	1911	PSU	O2-C2	-2.34	1.18	1.23
22	A2	746	PSU	O2-C2	-2.34	1.18	1.23
53	f2	8	4SU	C3'-C4'	-2.30	1.47	1.53
22	A2	2580	PSU	O4'-C1'	-2.30	1.40	1.43
22	A2	2251	OMG	C5-C4	-2.25	1.37	1.43
22	A2	1962	5MC	C6-C5	2.22	1.38	1.34
22	A2	746	PSU	O4'-C1'	-2.18	1.40	1.43
22	A2	2503	2MA	C5-C4	-2.17	1.37	1.43
22	A2	2445	2MG	C4-N3	-2.12	1.32	1.37
53	f2	8	4SU	O2'-C2'	-2.11	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	2069	G7M	C5-C6	-2.09	1.40	1.45
22	A2	1835	2MG	C4-N3	-2.03	1.32	1.37
22	A2	2580	PSU	C4-C5	-2.01	1.38	1.44
22	A2	2498	OMC	C5-C4	-2.00	1.38	1.42

All (146) 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
53	f2	8	4SU	C5-C4-N3	14.84	128.45	114.69
53	f2	8	4SU	C4-N3-C2	-12.97	114.73	127.34
22	A2	2449	H2U	O2-C2-N1	-11.49	108.68	123.11
53	f2	8	4SU	C2'-C1'-N1	-9.54	86.20	113.22
22	A2	1939	5MU	C4-N3-C2	-9.13	115.53	127.35
53	f2	55	PSU	C6-C5-C4	-9.10	111.83	118.20
53	f2	8	4SU	C5-C4-S4	-8.84	113.08	124.47
53	f2	8	4SU	C6-C5-C4	-8.57	112.53	119.95
22	A2	747	5MU	C4-N3-C2	-8.56	116.27	127.35
22	A2	747	5MU	C5M-C5-C4	8.48	128.10	118.77
22	A2	1939	5MU	N3-C2-N1	8.44	126.09	114.89
53	f2	54	5MU	O4-C4-C5	-8.35	115.22	124.90
22	A2	1939	5MU	C5-C6-N1	-8.33	114.77	123.34
53	f2	8	4SU	N3-C2-N1	8.26	125.86	114.89
22	A2	747	5MU	N3-C2-N1	8.22	125.80	114.89
22	A2	1939	5MU	C5M-C5-C4	8.09	127.67	118.77
22	A2	2449	H2U	O4-C4-N3	-7.92	107.72	120.28
53	f2	54	5MU	C5-C4-N3	7.44	121.66	115.31
22	A2	747	5MU	C5-C6-N1	-7.32	115.81	123.34
22	A2	2449	H2U	O2-C2-N3	-7.19	108.11	121.50
22	A2	1915	3TD	N1-C2-N3	6.99	121.65	116.14
22	A2	1939	5MU	C5-C4-N3	6.87	121.18	115.31
22	A2	747	5MU	C5M-C5-C6	-6.57	114.07	122.85
22	A2	2449	H2U	O4-C4-C5	-6.54	108.19	122.17
22	A2	1939	5MU	C5M-C5-C6	-6.51	114.16	122.85
22	A2	2030	6MZ	C9-N6-C6	-6.46	117.30	122.87
22	A2	747	5MU	C5-C4-N3	6.46	120.83	115.31
53	f2	54	5MU	C4-N3-C2	-6.43	119.02	127.35
22	A2	2449	H2U	N3-C2-N1	-6.07	110.24	116.65
22	A2	2580	PSU	N1-C2-N3	5.74	121.64	115.13
22	A2	2504	PSU	N1-C2-N3	5.72	121.61	115.13
22	A2	2457	PSU	N1-C2-N3	5.71	121.60	115.13
22	A2	2604	PSU	N1-C2-N3	5.62	121.50	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A2	955	PSU	N1-C2-N3	5.57	121.44	115.13
53	f2	55	PSU	O3'-C3'-C4'	5.57	127.14	111.05
22	A2	1917	PSU	N1-C2-N3	5.56	121.44	115.13
22	A2	2605	PSU	N1-C2-N3	5.56	121.42	115.13
22	A2	2552	OMU	N3-C2-N1	5.51	122.21	114.89
22	A2	1911	PSU	N1-C2-N3	5.51	121.37	115.13
53	f2	54	5MU	N3-C2-N1	5.45	122.12	114.89
22	A2	746	PSU	N1-C2-N3	5.43	121.28	115.13
53	f2	8	4SU	O2-C2-N1	-5.35	115.67	122.79
22	A2	2030	6MZ	C2-N1-C6	5.24	121.08	116.59
53	f2	8	4SU	O3'-C3'-C2'	5.22	128.71	111.82
22	A2	2030	6MZ	N3-C2-N1	-4.92	120.99	128.68
22	A2	1618	6MZ	C2-N1-C6	4.81	120.71	116.59
22	A2	2552	OMU	C4-N3-C2	-4.76	120.31	126.58
22	A2	1618	6MZ	C9-N6-C6	-4.75	118.78	122.87
22	A2	1618	6MZ	N3-C2-N1	-4.71	121.31	128.68
53	f2	8	4SU	C6-N1-C2	-4.66	115.03	120.99
53	f2	32	5MC	C5-C6-N1	-4.29	118.92	123.34
53	f2	55	PSU	C2'-C3'-C4'	-4.24	94.40	102.64
22	A2	1939	5MU	O2-C2-N1	-4.24	117.15	122.79
22	A2	1962	5MC	C5-C6-N1	-4.23	118.99	123.34
53	f2	55	PSU	N1-C2-N3	4.18	119.86	115.13
22	A2	2605	PSU	C4-N3-C2	-4.12	120.40	126.34
22	A2	2457	PSU	C4-N3-C2	-4.09	120.44	126.34
22	A2	746	PSU	C4-N3-C2	-4.06	120.50	126.34
22	A2	2604	PSU	C4-N3-C2	-4.05	120.50	126.34
22	A2	2504	PSU	C4-N3-C2	-4.04	120.51	126.34
22	A2	1939	5MU	O4-C4-N3	-4.00	112.44	120.12
22	A2	955	PSU	C4-N3-C2	-3.92	120.68	126.34
22	A2	1911	PSU	C4-N3-C2	-3.92	120.69	126.34
53	f2	55	PSU	O4'-C1'-C2'	-3.91	99.64	105.14
22	A2	1917	PSU	C4-N3-C2	-3.90	120.72	126.34
22	A2	2580	PSU	C4-N3-C2	-3.89	120.73	126.34
22	A2	747	5MU	O4-C4-N3	-3.87	112.69	120.12
53	f2	54	5MU	O4'-C4'-C3'	-3.74	97.72	105.11
53	f2	54	5MU	C3'-C2'-C1'	-3.68	94.44	101.43
34	M2	81	4D4	NE-CZ-NH2	-3.60	114.37	120.70
22	A2	1915	3TD	C4-N3-C2	-3.51	120.80	124.61
22	A2	747	5MU	O2-C2-N1	-3.46	118.19	122.79
53	f2	54	5MU	C2'-C1'-N1	-3.44	103.48	113.22
22	A2	745	1MG	C5-C6-N1	3.38	118.98	113.90
53	f2	54	5MU	O2'-C2'-C3'	3.34	122.62	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	f2	55	PSU	O2'-C2'-C3'	-3.33	101.05	111.82
53	f2	8	4SU	C3'-C2'-C1'	3.32	107.74	101.43
22	A2	2504	PSU	O2-C2-N1	-3.29	119.17	122.79
22	A2	955	PSU	O2-C2-N1	-3.24	119.23	122.79
22	A2	1835	2MG	C5-C6-N1	3.17	119.56	113.95
22	A2	2580	PSU	O2-C2-N1	-3.17	119.30	122.79
34	M2	81	4D4	NH1-CZ-NE	3.16	126.48	119.19
22	A2	2457	PSU	O2-C2-N1	-3.14	119.34	122.79
53	f2	54	5MU	O3'-C3'-C2'	3.13	121.93	111.82
22	A2	1911	PSU	O2-C2-N1	-3.05	119.44	122.79
22	A2	2552	OMU	O2-C2-N1	-3.04	118.74	122.79
22	A2	746	PSU	O2-C2-N1	-3.03	119.45	122.79
53	f2	55	PSU	O2'-C2'-C1'	3.02	118.44	111.23
22	A2	1917	PSU	O2-C2-N1	-3.01	119.48	122.79
22	A2	2445	2MG	C5-C6-N1	3.00	119.24	113.95
22	A2	747	5MU	C1'-N1-C6	-2.98	116.17	121.12
22	A2	747	5MU	O2-C2-N3	-2.95	116.01	121.50
22	A2	1939	5MU	C6-N1-C2	2.93	124.27	121.30
22	A2	2604	PSU	O2-C2-N1	-2.92	119.58	122.79
22	A2	2498	OMC	O2-C2-N3	-2.89	117.62	122.33
22	A2	2503	2MA	C5-C6-N1	2.86	118.95	114.02
22	A2	2251	OMG	C8-N7-C5	2.84	108.40	102.99
22	A2	2605	PSU	O2-C2-N1	-2.81	119.69	122.79
53	f2	54	5MU	C2'-C3'-C4'	2.75	107.99	102.64
53	f2	8	4SU	O2'-C2'-C3'	2.73	120.66	111.82
22	A2	1835	2MG	C8-N7-C5	2.73	108.19	102.99
22	A2	745	1MG	C8-N7-C5	2.73	108.19	102.99
53	f2	8	4SU	O4'-C1'-C2'	-2.73	100.70	106.64
22	A2	2445	2MG	C8-N7-C5	2.71	108.14	102.99
53	f2	8	4SU	C1'-N1-C2	2.70	122.46	117.57
53	f2	54	5MU	C5'-C4'-C3'	-2.69	105.10	115.18
22	A2	2552	OMU	C5-C6-N1	-2.67	117.33	121.81
22	A2	2030	6MZ	C4-C5-N7	-2.66	106.62	109.40
22	A2	2552	OMU	C5-C4-N3	2.62	118.76	114.84
53	f2	32	5MC	C5-C4-N3	-2.61	118.86	121.67
53	f2	55	PSU	O2-C2-N1	-2.56	119.97	122.79
22	A2	1939	5MU	O2-C2-N3	-2.55	116.75	121.50
53	f2	55	PSU	C4-N3-C2	-2.51	122.72	126.34
22	A2	2552	OMU	O4-C4-C5	-2.51	120.75	125.16
22	A2	2457	PSU	C5-C6-N1	-2.51	118.35	122.11
22	A2	2604	PSU	C5-C6-N1	-2.47	118.41	122.11
22	A2	746	PSU	C5-C6-N1	-2.46	118.42	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A2	2605	PSU	C5-C6-N1	-2.46	118.42	122.11
34	M2	81	4D4	CB-CA-C	-2.45	107.85	111.77
53	f2	8	4SU	C4'-O4'-C1'	2.44	114.86	109.47
22	A2	2251	OMG	C5-C6-N1	2.38	118.16	113.95
22	A2	1911	PSU	C5-C6-N1	-2.33	118.61	122.11
22	A2	2449	H2U	C5-C4-N3	-2.33	114.03	116.65
53	f2	8	4SU	O4'-C4'-C3'	-2.32	100.53	105.11
22	A2	2504	PSU	C5-C6-N1	-2.30	118.65	122.11
22	A2	745	1MG	O6-C6-C5	-2.26	120.18	124.19
53	f2	54	5MU	C5-C6-N1	-2.26	121.02	123.34
22	A2	1917	PSU	C5-C6-N1	-2.25	118.73	122.11
53	f2	32	5MC	CM5-C5-C6	-2.25	119.85	122.85
22	A2	2445	2MG	CM2-N2-C2	-2.24	118.91	123.86
22	A2	2580	PSU	C5-C6-N1	-2.21	118.79	122.11
22	A2	955	PSU	C5-C6-N1	-2.21	118.80	122.11
22	A2	1835	2MG	CM2-N2-C2	-2.20	119.00	123.86
22	A2	2580	PSU	O4'-C1'-C2'	2.19	108.23	105.14
22	A2	1618	6MZ	C4-C5-N7	-2.15	107.16	109.40
22	A2	2503	2MA	C8-N7-C5	2.15	107.08	102.99
22	A2	747	5MU	C6-N1-C2	2.13	123.45	121.30
34	M2	81	4D4	O-C-CA	-2.10	119.27	124.78
53	f2	55	PSU	C5'-C4'-C3'	2.08	122.97	115.18
53	f2	55	PSU	C4'-O4'-C1'	2.06	113.73	108.55
53	f2	54	5MU	O2-C2-N3	-2.06	117.67	121.50
53	f2	55	PSU	C3'-C2'-C1'	2.04	104.01	101.64
53	f2	54	5MU	C6-C5-C4	-2.02	116.34	118.03
22	A2	1962	5MC	C5-C4-N3	-2.02	119.50	121.67
22	A2	2251	OMG	C2-N1-C6	-2.01	121.40	125.10

There are no chirality outliers.

All (25) torsion outliers are listed below:

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
53	f2	55	PSU	C2'-C1'-C5-C4
53	f2	55	PSU	C2'-C1'-C5-C6
22	A2	2030	6MZ	O4'-C4'-C5'-O5'
22	A2	2030	6MZ	C3'-C4'-C5'-O5'
22	A2	2445	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	A2	2504	PSU	O4'-C4'-C5'-O5'
22	A2	2504	PSU	C3'-C4'-C5'-O5'
53	f2	55	PSU	C3'-C4'-C5'-O5'
53	f2	55	PSU	O4'-C4'-C5'-O5'
22	A2	2445	2MG	O4'-C4'-C5'-O5'
34	M2	81	4D4	OB-CB-CG-CD
25	D2	150[A]	MEQ	C-CA-CB-CG
34	M2	81	4D4	CA-CB-CG-CD
25	D2	150[A]	MEQ	OE1-CD-CG-CB
25	D2	150[A]	MEQ	NE2-CD-CG-CB
53	f2	55	PSU	O4'-C1'-C5-C4
22	A2	1962	5MC	C2'-C1'-N1-C6
22	A2	2503	2MA	O4'-C4'-C5'-O5'
22	A2	1962	5MC	O4'-C1'-N1-C6
22	A2	746	PSU	O4'-C1'-C5-C6
22	A2	2069	G7M	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)

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	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
54	DI0	A2	3001	-	-	10/70/121/121	0/3/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A2	3001	DI0	CAF-CAE	-5.60	1.39	1.51
54	A2	3001	DI0	OBI-CAG	-4.12	1.33	1.43
54	A2	3001	DI0	OAU-CBG	-3.41	1.38	1.44
54	A2	3001	DI0	OAY-CAC	-3.13	1.35	1.43
54	A2	3001	DI0	CBC-CBB	2.86	1.58	1.54
54	A2	3001	DI0	OAU-CAB	-2.79	1.34	1.41
54	A2	3001	DI0	CAP-CAH	2.66	1.60	1.55
54	A2	3001	DI0	CAI-CAK	2.49	1.57	1.54
54	A2	3001	DI0	CAD-CAW	-2.49	1.50	1.54
54	A2	3001	DI0	OBJ-CAP	-2.28	1.40	1.44
54	A2	3001	DI0	OBL-CAX	-2.25	1.38	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A2	3001	DI0	OAL-CAW-CBT	4.88	116.70	107.40
54	A2	3001	DI0	CBT-CAW-CAD	-4.69	106.31	115.20
54	A2	3001	DI0	OBK-CAN-CAX	4.22	110.07	103.81
54	A2	3001	DI0	CAP-CAH-CAJ	-3.35	109.30	114.05
54	A2	3001	DI0	CBR-CAP-CBC	-2.75	106.45	111.09
54	A2	3001	DI0	CCB-OBK-CAN	-2.68	111.95	117.55
54	A2	3001	DI0	CBV-CBB-CBC	-2.64	106.45	112.45
54	A2	3001	DI0	CBP-CAJ-CAC	-2.51	106.89	111.40
54	A2	3001	DI0	CAF-CAC-CAJ	-2.37	106.20	113.05
54	A2	3001	DI0	OBI-CAG-CAO	-2.35	105.59	109.77
54	A2	3001	DI0	OBJ-CAP-CAH	2.22	111.80	107.59
54	A2	3001	DI0	OBK-CAN-CAT	-2.22	109.41	112.96
54	A2	3001	DI0	OAY-CAR-CAT	2.13	112.68	109.01
54	A2	3001	DI0	CBO-CAI-CAA	-2.12	107.97	112.94
54	A2	3001	DI0	CBO-CAI-CAK	-2.11	109.52	112.02
54	A2	3001	DI0	OAU-CAB-CAG	-2.08	105.95	110.35
54	A2	3001	DI0	OBK-CAN-CBQ	-2.07	107.48	110.92
54	A2	3001	DI0	CAN-CAX-CAZ	-2.06	107.98	111.14
54	A2	3001	DI0	OAM-CAH-CAJ	-2.04	108.48	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A2	3001	DI0	OAM-CAB-OAU	-2.03	105.02	110.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

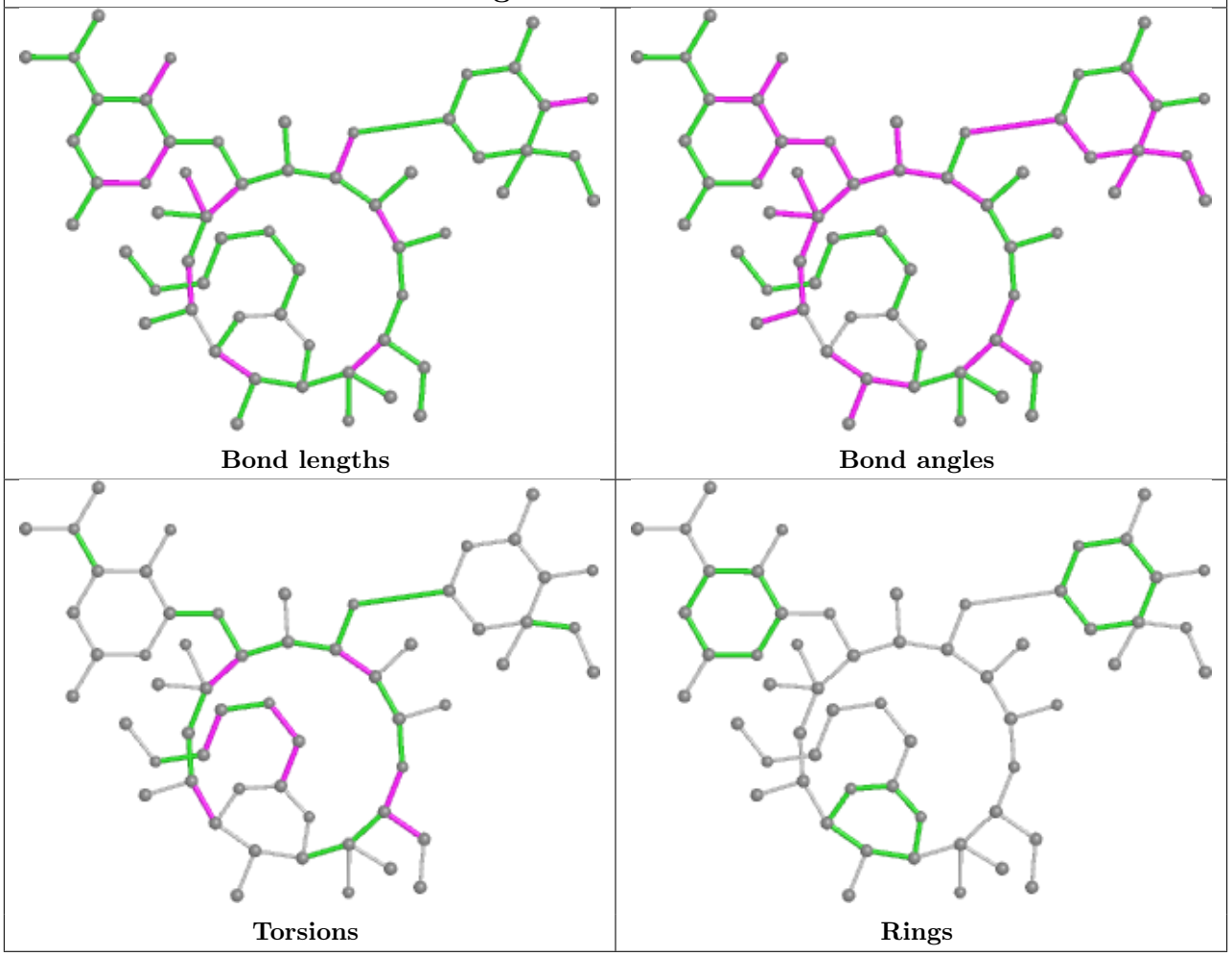
Mol	Chain	Res	Type	Atoms
54	A2	3001	DI0	NAQ-CBA-CBS-OBW
54	A2	3001	DI0	NAQ-CAK-CBB-CBC
54	A2	3001	DI0	CAJ-CAH-CAP-OBJ
54	A2	3001	DI0	OBX-CCC-CCD-OBW
54	A2	3001	DI0	OAL-CAW-CBT-CCF
54	A2	3001	DI0	CAD-CAW-OAL-CAE
54	A2	3001	DI0	CBA-CBS-OBW-CCD
54	A2	3001	DI0	CAJ-CAC-CAF-CBN
54	A2	3001	DI0	CAD-CAW-CBT-CCF
54	A2	3001	DI0	NAQ-CAK-CBB-CBV

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.

Ligand DI0 A2 3001



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

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	P	11.25

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-10656. 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

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

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

6 Map analysis

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

6.1 Map-value distribution

This section was not generated.

6.2 Volume estimate versus contour level

This section was not generated.

6.3 Rotationally averaged power spectrum

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

This section was not generated.