

wwPDB EM Validation Summary Report (i)

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).

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Deposited on : 2020-02-03

Resolution : 2.66 Å(reported)

Based on initial model : 4YBB

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

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)

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		1		AltConf	Trace		
1	A1	1523	Total 32681	C 14576	N 5998	O 10584	P 1523	0	0

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

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

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

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

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

Mol	Chain	Residues		Ato	oms			AltConf	Trace
4	D1	205	Total 1643	C 1026	N 315	O 298	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	O 211	S 6	0	0

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

\mathbf{Mol}	Chain	Residues		At	oms			AltConf	Trace
6	F1	106	Total 862		N 156	O 154	S 7	0	0



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

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	C1	151	Total	С	N	О	S	0	0
'	GI	101	1182	735	227	216	4		

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
0	Ш1	129	Total	С	N	О	S	0	0
0	111	129	979	616	173	184	6		U

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

Mol	Chain	Residues		At	oms			AltConf	Trace
9	I1	127	Total 1022	C 634	N 206	O 179	S 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	O 145	S 1	0	0

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

Mol	Chain	Residues		Atoms					Trace
11	K1	117	Total 877	C 540	N 174	O 160	S 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	O 162	S 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	_	N 178	O 157	S 3	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
1.4	N1	100	Total	С	N	О	S	0	0
14	111	100	805	499	164	139	3	0	

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

Mol	Chain	Residues		At	oms			AltConf	Trace
15	O1	88	Total	С	N	О	S	0	0
10	01		714	439	144	130	1		

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

Mol	Chain	Residues		At	oms			AltConf	Trace
16	D1	82	Total	С	N	О	S	0	0
10	11	02	649	406	128	114	1	0	U

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

Mol	Chain	Residues		At	oms			AltConf	Trace
17	O1	90	Total	С	N	О	S	0	0
11	Q_1	80	649	411	121	114	3	U	U

• 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
10	C1	79	Total	С	N	О	S	0	0
19	51	19	638	408	120	108	2	U	U

• 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	O 115	S 3	0	0

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



Mol	Chain	Residues		Ato	ms			AltConf	Trace
21	TT1	56	Total	С	N	О	S	0	0
21	01	90	465	290	96	78	1	U	U

• 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	P 2899	3	0

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

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

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

Mol	Chain	Residues		Ato	oms			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	O 294	S 4	1	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	E2	201	Total 1552	C 974	N 283	O 290	S 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	Co	176	Total	С	N	О	S	0	0
20	G2	170	1323	832	243	246	2	0	

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	Н9	135	Total	С	N	О	S	0	0
23	112	155	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		At	oms	AltConf	Trace		
30	I2	134	Total	C	N	0	S	0	0
			979	619	169	185	О		

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	J2	142	Total 1129	C 714	N 212	O 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	O 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	S 2	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	Atoms					AltConf	Trace
25	N2	125	Total	С	N	О	S	0	0
35	11/2	120	993	613	202	173	5	U	U

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	Ω^2	117	Total	С	N	О	S	0	0
30	02	111	900	557	179	163	1	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
27	DΩ	114	Total	С	N	О	S	0	0
31	1 2	114	917	574	179	163	1	0	U

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

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

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	D9	109	Total	С	N	О	S	0	0
39	$ \Lambda^{2} $	103	816	516	153	145	2	U	U

• 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	O 156	S 3	0	0

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



Mol	Chain	Residues		At	oms	AltConf	Trace		
//1	ТЭ	93	Total	С	N	О	S	0	0
41	12	90	739	466	139	132	2	0	U

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

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
42	110	102	Total	С	N	О	0	0
42	02	102	780	492	146	142	0	0

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

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

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
4.4	W2	76	Total	С	N	О	S	1	0
44	VV Z	10	580	359	117	103	1	1	U

• 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	S 2	0	0

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

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
16	V9	62	Total	С	N	О	S	0	0
46	1 2	02	501	308	98	94	1	U	U

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

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
17	79	58	Total	С	N	О	S	9	0
41	212	30	449	281	87	79	2	2	U

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



Mol	Chain	Residues		\mathbf{Atc}	$\mathbf{m}\mathbf{s}$	AltConf	Trace		
48	9.9	56	Total	С	N	О	S	0	0
40	a2	56	444	269	94	80	1	U	0

 \bullet Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ns	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.

Mo	Chain	Residues		Ato	$\mathbf{m}\mathbf{s}$	AltConf	Trace		
50	c2	46	Total 377	C 228	N 90	O 57	S 2	0	0

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

	Mol	Chain	Residues		Ato	oms	AltConf	Trace		
	51 d2	49	64	Total	С	N	О	S	0	0
		02		504	323	105	74	2		

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

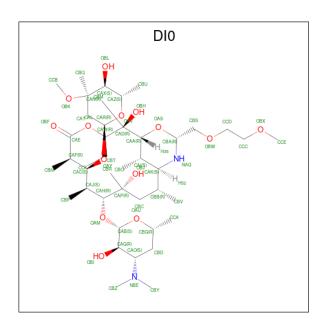
Mol	Chain	Residues		Ato	$\mathbf{m}\mathbf{s}$	AltConf	Trace		
52	e2	38	Total 302	C 185	N 65	O 48	S 4	0	0

• 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	P 76	S 1	0	0

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





Mol	Chain	Residues	A	AltConf			
54	A2	1	Total	С	N	O	0
0.1		-	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	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	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 (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)

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	В	ond leng	gths	В	ond ang	gles
MOI	туре	Chain	nes	Lilik	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%)



Mal	T	Clasies	Das	T 2 1-	В	ond leng	$_{ m gths}$	В	ond ang	gles
Mol	Type	Chain	Res	Link	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

The worst 5 of 181 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
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

The worst 5 of 146 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
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

There are no chirality outliers.

5 of 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

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	Tuno	Chain	Ros	Link	B	ond leng	gths	В	ond ang	gles
IVIOI	$oxed{ ext{Type} ext{Chain} ext{Re}}$	nes	LIIIK	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	\mathbf{Type}	Chain	Res	Link	Chirals	Torsions	Rings
54	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	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	Ideal(A)
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

The worst 5 of 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

There are no chirality outliers.

5 of 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

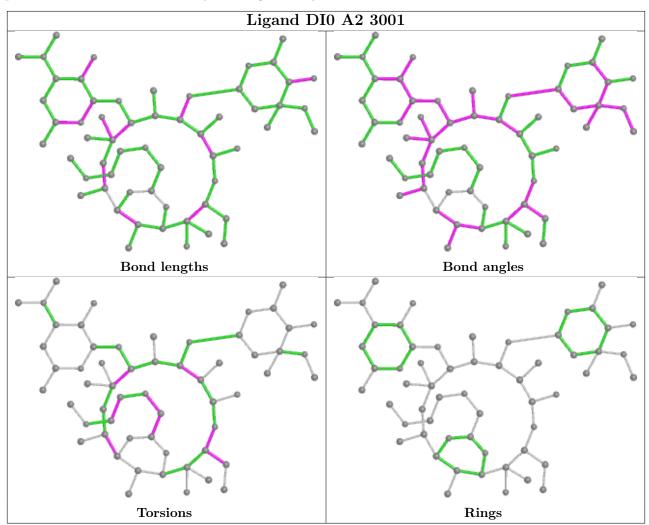
There are no ring outliers.

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

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



5 Map visualisation (i)

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 (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.

