



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 08:59 AM EST

PDB ID : 6PCT
EMDB ID : EMD-20307
Title : E. coli 50S ribosome bound to compound 41q
Authors : Pellegrino, J.; Lee, D.J.; Fraser, J.S.; Seiple, I.B.
Deposited on : 2019-06-18
Resolution : 2.80 Å(reported)

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 ⓘ 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:

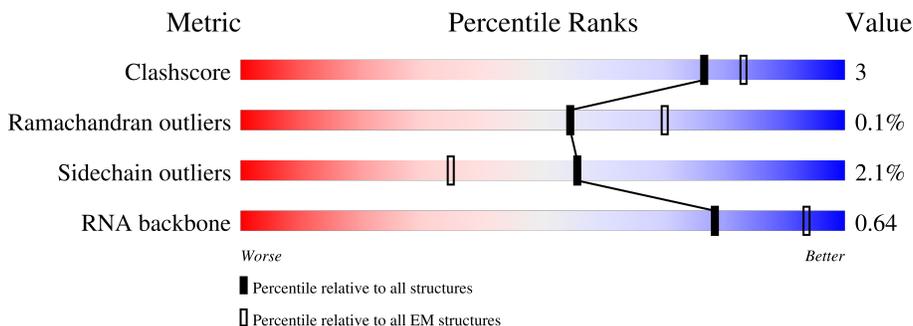
EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	I	2904	
2	J	118	
3	K	271	
4	L	144	
5	M	201	
6	N	209	
7	O	142	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 72198 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	I	2897	62206	27757	11443	20109	2897	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	J	118	2529	1126	464	821	118	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L15.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

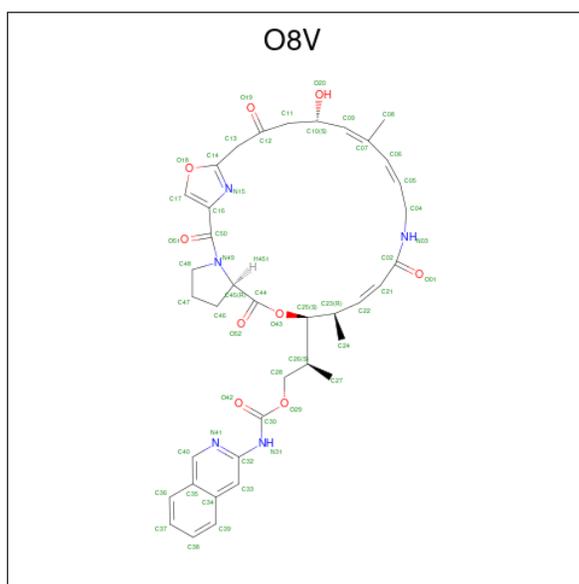
- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	206	1542	965	284	289	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

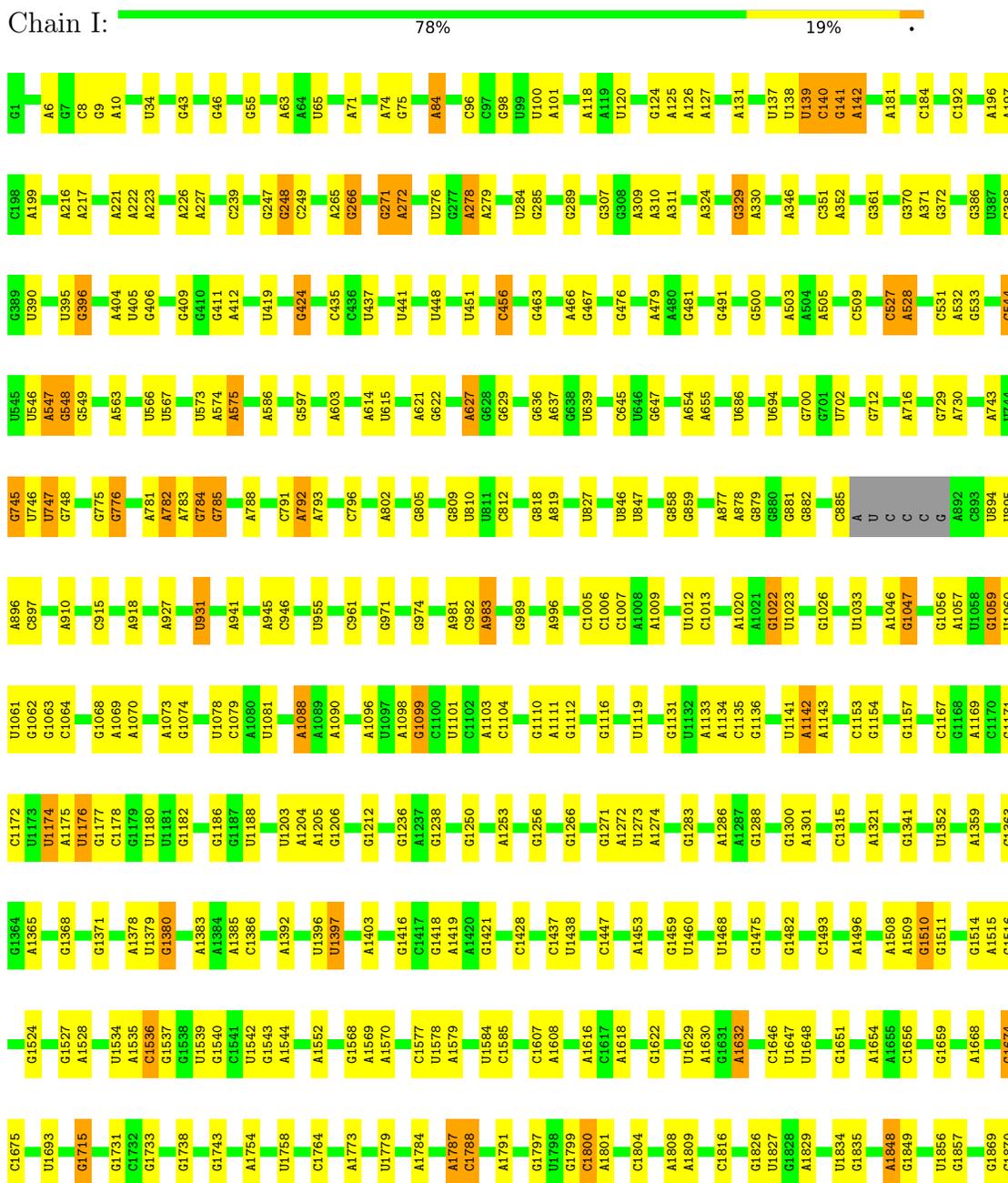
- Molecule 8 is (2S)-2-[(3S,4R,5E,10E,12E,14S,26aR)-14-hydroxy-4,12-dimethyl-1,7,16,22-tetraoxo-4,7,8,9,14,15,16,17,24,25,26,26a-dodecahydro-1H,3H,22H-21,18-(azeno)pyrrolo[2,1-c][1,8,4,19]dioxadiazacyclotetracosin-3-yl]propyl isoquinolin-3-ylcarbamate (three-letter code: O8V) (formula: C₃₈H₄₃N₅O₉) (labeled as "Ligand of Interest" by depositor).



3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA



Chain M:  86% 14%



- Molecule 6: 50S ribosomal protein L3

Chain N:  89% 10%



- Molecule 7: 50S ribosomal protein L13

Chain O:  82% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20644	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 ($e^-/\text{\AA}^2$)	83	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, OMG, 6MZ, 2MG, OMU, 5MC, O8V, OMC, 1MG, G7M, 3TD, PSU, 5MU

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.27	0/69165	0.68	0/107896
2	J	0.22	0/2828	0.66	0/4410
3	K	0.33	0/2122	0.49	0/2852
4	L	0.27	0/1062	0.47	0/1413
5	M	0.33	0/1571	0.46	0/2113
6	N	0.31	0/1561	0.49	0/2097
7	O	0.28	0/1152	0.43	0/1551
All	All	0.27	0/79461	0.66	0/122332

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	62206	0	31305	220	0
2	J	2529	0	1281	6	0
3	K	2083	0	2154	33	0
4	L	1053	0	1129	11	0
5	M	1552	0	1618	20	0
6	N	1542	0	1593	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	1129	0	1162	20	0
8	I	104	0	0	3	0
All	All	72198	0	40242	288	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 288 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1799:G:OP2	3:K:270:ARG:NH1	1.96	0.99
1:I:137:U:O2'	1:I:140:C:N4	2.03	0.92
1:I:1779:U:OP2	1:I:1784:A:N6	2.05	0.90
1:I:1911:PSU:O2'	1:I:1912:A:OP1	1.89	0.89
3:K:225:MET:O	3:K:229:ASP:HB2	1.72	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	269/271 (99%)	242 (90%)	26 (10%)	1 (0%)	34	66
4	L	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
5	M	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
6	N	202/209 (97%)	191 (95%)	11 (5%)	0	100	100
7	O	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
All	All	952/967 (98%)	891 (94%)	60 (6%)	1 (0%)	54	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	226	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	216/216 (100%)	210 (97%)	6 (3%)	43	77
4	L	103/103 (100%)	101 (98%)	2 (2%)	57	85
5	M	165/165 (100%)	161 (98%)	4 (2%)	49	81
6	N	161/164 (98%)	160 (99%)	1 (1%)	86	96
7	O	116/116 (100%)	113 (97%)	3 (3%)	46	79
All	All	761/764 (100%)	745 (98%)	16 (2%)	56	84

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	O	86	GLN
7	O	64	VAL
5	M	17	THR
6	N	118	PHE
4	L	94	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	41	GLN
7	O	86	GLN
7	O	128	ASN
3	K	226	ASN
3	K	153	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2891/2904 (99%)	349 (12%)	8 (0%)
2	J	117/118 (99%)	7 (5%)	0
All	All	3008/3022 (99%)	356 (11%)	8 (0%)

5 of 356 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	10	A
1	I	34	U
1	I	43	G
1	I	46	G
1	I	63	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	2602	A
1	I	2481	G
1	I	1911	PSU
1	I	1787	A
1	I	2425	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

21 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
1	5MU	I	1939	1	19,22,23	1.02	2 (10%)	28,32,35	2.08	6 (21%)
1	PSU	I	2457	1	18,21,22	0.94	1 (5%)	22,30,33	1.81	4 (18%)
1	PSU	I	2504	1	18,21,22	0.94	1 (5%)	22,30,33	1.78	3 (13%)
1	1MG	I	745	1	18,26,27	1.23	2 (11%)	19,39,42	1.28	3 (15%)
1	PSU	I	2580	1	18,21,22	0.98	1 (5%)	22,30,33	1.81	3 (13%)
1	6MZ	I	1618	1	18,25,26	1.04	2 (11%)	16,36,39	1.95	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	I	2498	1	19,22,23	0.87	1 (5%)	26,31,34	0.97	2 (7%)
1	5MC	I	1962	1	18,22,23	0.84	1 (5%)	26,32,35	1.14	2 (7%)
1	2MG	I	1835	1	18,26,27	1.23	2 (11%)	16,38,41	1.25	2 (12%)
1	2MA	I	2503	1	17,25,26	0.82	1 (5%)	17,37,40	0.97	1 (5%)
1	OMG	I	2251	1	18,26,27	1.22	2 (11%)	19,38,41	1.46	4 (21%)
1	OMU	I	2552	1	19,22,23	0.96	1 (5%)	26,31,34	1.85	6 (23%)
1	2MG	I	2445	1,5	18,26,27	1.27	2 (11%)	16,38,41	1.24	2 (12%)
1	5MU	I	747	1	19,22,23	1.00	2 (10%)	28,32,35	2.07	7 (25%)
1	PSU	I	746	1	18,21,22	0.99	1 (5%)	22,30,33	1.68	3 (13%)
1	PSU	I	1911	1	18,21,22	0.88	0	22,30,33	1.87	4 (18%)
1	G7M	I	2069	1	20,26,27	0.92	1 (5%)	17,39,42	0.51	0
1	3TD	I	1915	1	18,22,23	0.91	1 (5%)	22,32,35	1.65	2 (9%)
1	PSU	I	1917	1	18,21,22	0.86	0	22,30,33	1.82	3 (13%)
1	PSU	I	2605	1	18,21,22	0.92	1 (5%)	22,30,33	1.82	3 (13%)
1	PSU	I	955	1	18,21,22	0.95	1 (5%)	22,30,33	1.81	4 (18%)

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
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
1	1MG	I	745	1	-	0/3/25/26	0/3/3/3
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	I	1618	1	-	2/5/27/28	0/3/3/3
1	OMC	I	2498	1	-	3/9/27/28	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	2MG	I	1835	1	-	0/5/27/28	0/3/3/3
1	2MA	I	2503	1	-	2/3/25/26	0/3/3/3
1	OMG	I	2251	1	-	0/5/27/28	0/3/3/3
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	2MG	I	2445	1,5	-	2/5/27/28	0/3/3/3
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	PSU	I	746	1	-	1/7/25/26	0/2/2/2
1	PSU	I	1911	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	I	2069	1	-	1/3/25/26	0/3/3/3
1	3TD	I	1915	1	-	5/7/25/26	0/2/2/2
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2445	2MG	C5-C6	-2.90	1.41	1.47
1	I	1835	2MG	C5-C6	-2.89	1.41	1.47
1	I	2251	OMG	C5-C6	-2.85	1.41	1.47
1	I	2069	G7M	C8-N9	2.81	1.38	1.33
1	I	2445	2MG	C8-N7	-2.78	1.30	1.35

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1915	3TD	N1-C2-N3	5.96	120.84	116.14
1	I	1939	5MU	C4-N3-C2	-5.45	120.29	127.35
1	I	747	5MU	C4-N3-C2	-5.38	120.39	127.35
1	I	1911	PSU	N1-C2-N3	5.26	121.09	115.13
1	I	1618	6MZ	C2-N1-C6	5.17	121.02	116.59

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1618	6MZ	C5-C6-N6-C9
1	I	1618	6MZ	N1-C6-N6-C9
1	I	1911	PSU	C3'-C4'-C5'-O5'
1	I	1915	3TD	O4'-C1'-C5-C4
1	I	1915	3TD	C2'-C1'-C5-C6

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	2504	PSU	1	0
1	I	745	1MG	1	0
1	I	2498	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	1962	5MC	1	0
1	I	2503	2MA	4	0
1	I	2251	OMG	1	0
1	I	1911	PSU	4	0
1	I	1915	3TD	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
8	O8V	I	3001[B]	-	52,56,56	0.99	1 (1%)	63,77,77	0.99	4 (6%)
8	O8V	I	3001[A]	-	52,56,56	0.98	1 (1%)	63,77,77	1.09	6 (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
8	O8V	I	3001[B]	-	-	4/51/67/67	0/4/5/5
8	O8V	I	3001[A]	-	-	7/51/67/67	0/4/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	3001[B]	O8V	C16-C50	-2.82	1.45	1.50
8	I	3001[A]	O8V	C16-C50	-2.68	1.46	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	3001[A]	O8V	O29-C30-N31	3.84	115.59	109.32
8	I	3001[B]	O8V	C44-C45-N49	3.41	118.96	112.07
8	I	3001[A]	O8V	C44-C45-N49	3.35	118.84	112.07
8	I	3001[A]	O8V	C28-O29-C30	2.67	121.47	116.06
8	I	3001[B]	O8V	C25-O43-C44	2.40	121.90	117.78

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

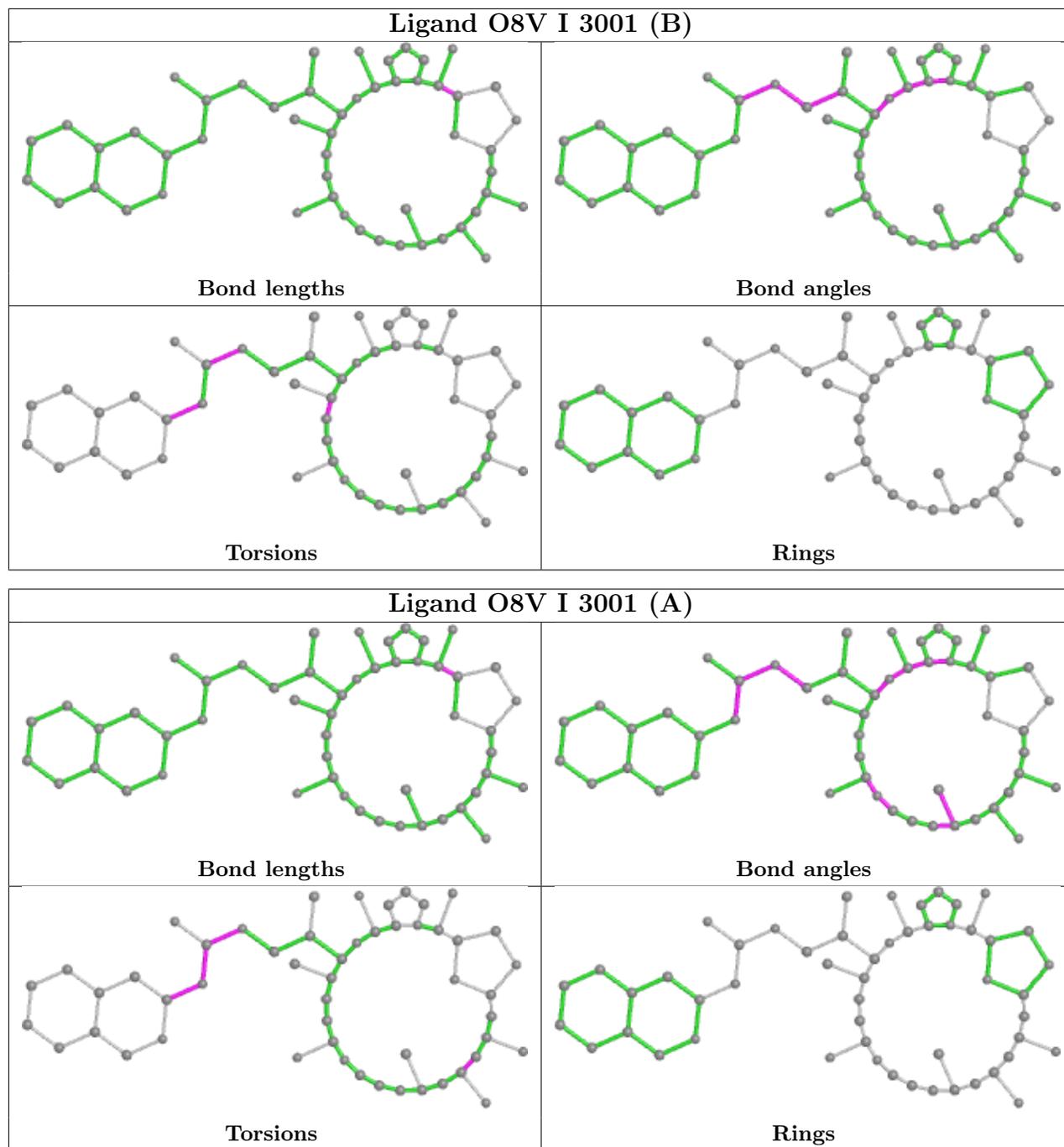
Mol	Chain	Res	Type	Atoms
8	I	3001[A]	O8V	N31-C30-O29-C28
8	I	3001[A]	O8V	O42-C30-O29-C28
8	I	3001[A]	O8V	C33-C32-N31-C30
8	I	3001[A]	O8V	N41-C32-N31-C30
8	I	3001[B]	O8V	C33-C32-N31-C30

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	3001[B]	O8V	2	0
8	I	3001[A]	O8V	1	0

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 than 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.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.