



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2022 – 05:19 PM EST

PDB ID : 1G5L
Title : CO(III)-BLEOMYCIN-OOH BOUND TO AN OLIGONUCLEOTIDE CONTAINING A PHOSPHOGLYCOLATE LESION
Authors : Hoehn, S.T.; Junker, H.-D.; Bunt, R.C.; Turner, C.J.; Stubbe, J.
Deposited on : 2000-11-01

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

2 Ensemble composition and analysis

This entry contains 10 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 988 atoms, of which 371 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*CP*CP*AP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	A	6	187	58	67	26	31	5	0

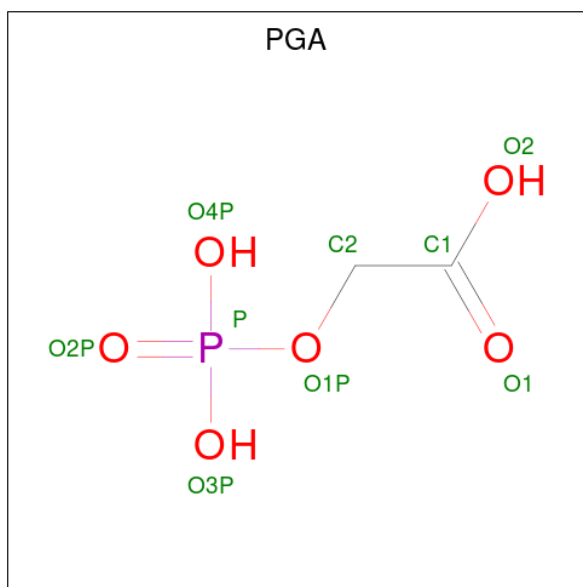
- Molecule 2 is a DNA chain called 5'-D(P*AP*CP*TP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
2	B	6	194	59	68	25	36	6	0

- Molecule 3 is a DNA chain called 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
3	C	13	410	126	149	45	78	12	0

- Molecule 4 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: C₂H₅O₆P).



Mol	Chain	Residues	Atoms				
			Total	C	H	O	P
4	A	1	10	2	2	5	1

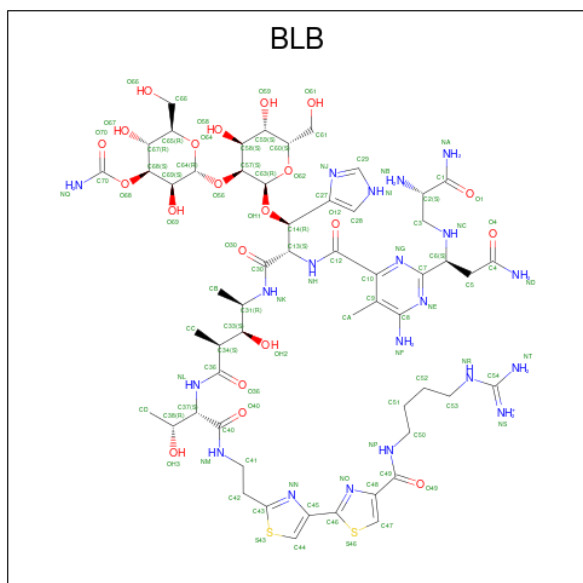
- Molecule 5 is COBALT (III) ION (three-letter code: 3CO) (formula: Co).

Mol	Chain	Residues	Atoms	
5	B	1	Total	Co
			1	1

- Molecule 6 is OXYGEN ATOM (three-letter code: O) (formula: O).

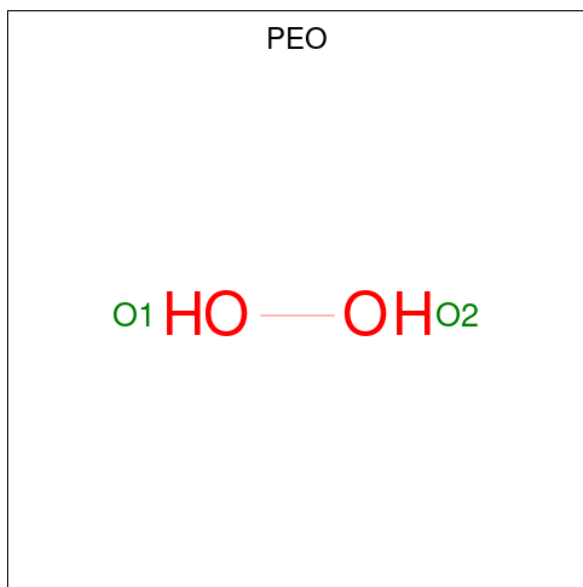
Mol	Chain	Residues	Atoms	
6	B	1	Total	O
			1	1

- Molecule 7 is BLEOMYCIN B2 (three-letter code: BLB) (formula: C₅₅H₈₅N₂₀O₂₁S₂).



Mol	Chain	Residues	Atoms					
7	C	1	Total	C	H	N	O	S
			182	55	84	20	21	2

- Molecule 8 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



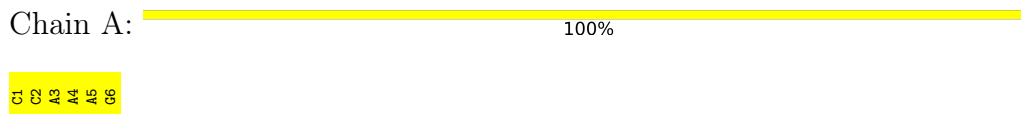
Mol	Chain	Residues	Atoms		
			Total	H	O
8	C	1	3	1	2

4 Residue-property plots

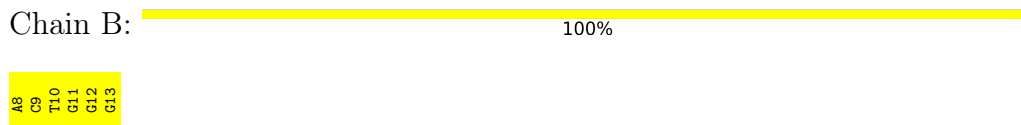
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

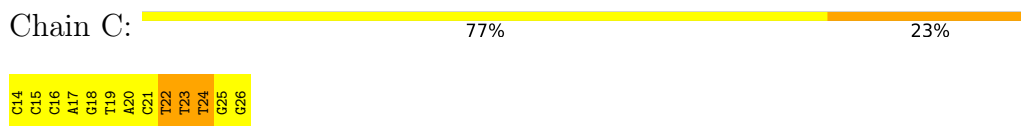
- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'



- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'



- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

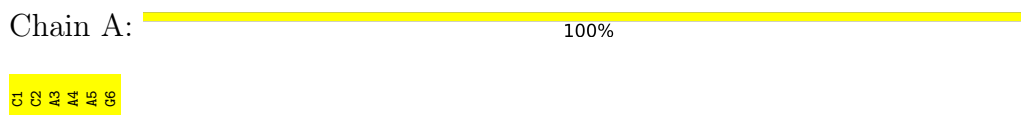


4.2 Scores per residue for each member of the ensemble


Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'




- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  8% 62% 31%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26


4.2.2 Score per residue for model 2

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%


C1
C2
A3
A4
A5
G6

- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  85% 15%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26


4.2.3 Score per residue for model 3

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%


C1
C2
A3
A4
A5
G6

- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

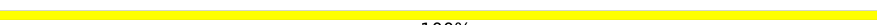
- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  77% 23%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26

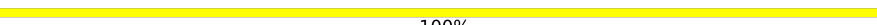
4.2.4 Score per residue for model 4

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%


C1
C2
A3
A4
A5
G6

- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

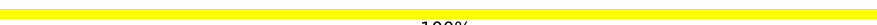
- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  85% 15%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26


4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%


C1
C2
A3
A4
A5
G6

- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  67% 33%

A8
C9
T10
G11
G12
G13

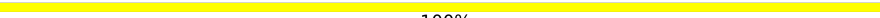
- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  69% 31%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26

4.2.6 Score per residue for model 6

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%



C1
C2
A3
A4
A5
G6

- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  77%  23%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26

4.2.7 Score per residue for model 7

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%



C1
C2
A3
A4
A5
G6

- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

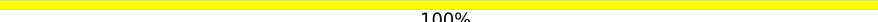
- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  77%  23%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26

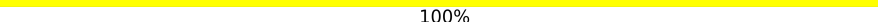
4.2.8 Score per residue for model 8

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%

C1
C2
A3
A4
A5
G6

- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

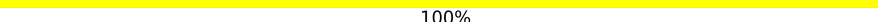
- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  69% 31%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26

4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%


C1
C2
A3
A4
A5
G6

- Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

- Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  8% 69% 23%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26

4.2.10 Score per residue for model 10

- Molecule 1: 5'-D(*CP*CP*AP*AP*AP*G)-3'

Chain A:  100%


C1
C2
A3
A4
A5
G6

• Molecule 2: 5'-D(P*AP*CP*TP*GP*GP*G)-3'

Chain B:  100%

A8
C9
T10
G11
G12
G13

• Molecule 3: 5'-D(*CP*CP*CP*AP*GP*TP*AP*CP*TP*TP*TP*GP*G)-3'

Chain C:  8% 62% 31%

C14
C15
C16
A17
G18
T19
A20
C21
T22
T23
T24
G25
G26

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *all calculated structures submitted*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: O, 3CO, BLB, PGA, PEO

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 (average) 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	A	1.68±0.03	2±1/135 (1.8± 0.6%)	2.43±0.06	11±1/206 (5.3± 0.6%)
2	B	1.77±0.04	1±1/141 (0.8± 0.4%)	2.67±0.06	16±2/216 (7.5± 0.9%)
3	C	1.71±0.04	2±1/291 (0.7± 0.2%)	3.33±0.04	37±3/447 (8.3± 0.7%)
All	All	1.72	55/5670 (1.0%)	2.98	642/8690 (7.4%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	17	DA	N9-C4	6.65	1.41	1.37	9	10
2	B	8	DA	N9-C4	6.03	1.41	1.37	9	8
3	C	20	DA	N9-C4	5.74	1.41	1.37	7	7
1	A	5	DA	N9-C4	5.71	1.41	1.37	2	8
1	A	3	DA	N9-C4	5.64	1.41	1.37	1	8
2	B	12	DG	N7-C5	-5.63	1.35	1.39	3	1
2	B	8	DA	P-O5'	-5.63	1.54	1.59	5	1
1	A	4	DA	N9-C4	5.58	1.41	1.37	7	7
3	C	18	DG	C5-C6	-5.21	1.37	1.42	9	1
3	C	23	DT	C5-C7	-5.17	1.47	1.50	9	1
3	C	17	DA	O4'-C1'	-5.11	1.36	1.42	5	1
1	A	6	DG	C5-C6	-5.06	1.37	1.42	7	1
2	B	12	DG	C5-C6	-5.02	1.37	1.42	3	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	24	DT	C6-C5-C7	-23.39	108.87	122.90	9	10
3	C	22	DT	C6-C5-C7	-21.75	109.85	122.90	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	24	DT	C4-C5-C7	19.53	130.72	119.00	9	10
3	C	22	DT	C4-C5-C7	18.00	129.80	119.00	3	10
3	C	20	DA	P-O3'-C3'	12.65	134.88	119.70	1	7
3	C	23	DT	C6-C5-C7	-12.21	115.58	122.90	7	10
3	C	17	DA	N1-C6-N6	11.65	125.59	118.60	4	10
3	C	22	DT	P-O3'-C3'	11.35	133.32	119.70	2	10
3	C	21	DC	P-O3'-C3'	10.77	132.62	119.70	2	6
2	B	8	DA	N1-C6-N6	10.60	124.96	118.60	9	10
3	C	15	DC	P-O3'-C3'	10.55	132.37	119.70	2	6
2	B	11	DG	N3-C2-N2	10.50	127.25	119.90	7	10
1	A	6	DG	N3-C2-N2	10.07	126.95	119.90	7	10
3	C	21	DC	O4'-C1'-N1	9.87	114.91	108.00	7	5
3	C	14	DC	O4'-C1'-N1	9.77	114.84	108.00	6	5
2	B	13	DG	N3-C2-N2	9.72	126.71	119.90	2	10
2	B	12	DG	N3-C2-N2	9.71	126.69	119.90	6	10
3	C	19	DT	C6-C5-C7	-9.71	117.08	122.90	1	10
2	B	9	DC	O4'-C1'-N1	9.52	114.67	108.00	5	8
3	C	18	DG	C5-C6-O6	-9.35	122.99	128.60	9	8
1	A	1	DC	O4'-C1'-N1	9.30	114.51	108.00	9	10
1	A	5	DA	N1-C6-N6	9.11	124.06	118.60	8	8
3	C	24	DT	P-O3'-C3'	8.79	130.25	119.70	9	10
2	B	8	DA	O4'-C1'-N9	-8.76	101.87	108.00	9	6
1	A	3	DA	P-O3'-C3'	8.48	129.88	119.70	2	9
3	C	14	DC	P-O3'-C3'	8.43	129.81	119.70	8	3
2	B	12	DG	P-O3'-C3'	8.34	129.71	119.70	7	4
3	C	18	DG	O4'-C1'-N9	-8.28	102.20	108.00	8	8
3	C	26	DG	N3-C2-N2	8.26	125.69	119.90	1	10
2	B	10	DT	C6-C5-C7	-8.16	118.00	122.90	7	10
3	C	18	DG	N1-C6-O6	8.07	124.74	119.90	9	2
3	C	22	DT	O4'-C4'-C3'	8.05	110.83	106.00	8	4
3	C	23	DT	C4-C5-C7	8.03	123.82	119.00	1	10
3	C	17	DA	C5-C6-N6	-7.90	117.38	123.70	4	5
2	B	9	DC	N3-C4-N4	7.81	123.47	118.00	4	6
1	A	2	DC	N1-C2-O2	7.77	123.56	118.90	4	10
2	B	9	DC	N3-C4-C5	-7.75	118.80	121.90	9	10
3	C	14	DC	N3-C4-C5	-7.59	118.86	121.90	1	10
3	C	19	DT	C4-C5-C7	7.57	123.54	119.00	8	8
1	A	4	DA	N1-C6-N6	7.54	123.12	118.60	4	10
2	B	8	DA	C5-C6-N6	-7.45	117.74	123.70	9	5
3	C	25	DG	N3-C2-N2	7.38	125.06	119.90	4	9
3	C	17	DA	P-O3'-C3'	7.35	128.52	119.70	6	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	20	DA	O4'-C1'-C2'	-7.33	100.04	105.90	2	4
3	C	20	DA	O4'-C1'-N9	-7.28	102.90	108.00	6	1
3	C	16	DC	N1-C2-O2	7.20	123.22	118.90	2	8
3	C	15	DC	N1-C2-O2	7.20	123.22	118.90	4	10
3	C	15	DC	N3-C2-O2	-7.17	116.88	121.90	4	8
3	C	21	DC	C1'-O4'-C4'	-7.12	102.98	110.10	5	6
3	C	18	DG	C8-N9-C4	-7.04	103.58	106.40	7	8
3	C	19	DT	O4'-C1'-C2'	-6.95	100.34	105.90	7	8
3	C	21	DC	O4'-C1'-C2'	-6.88	100.40	105.90	6	6
3	C	16	DC	P-O3'-C3'	6.85	127.92	119.70	9	6
1	A	5	DA	P-O3'-C3'	6.70	127.74	119.70	6	3
2	B	12	DG	C8-N9-C4	-6.63	103.75	106.40	3	4
2	B	13	DG	C8-N9-C4	-6.55	103.78	106.40	4	4
3	C	23	DT	O4'-C4'-C3'	6.50	109.90	106.00	2	10
3	C	15	DC	C6-N1-C2	-6.49	117.71	120.30	1	7
2	B	11	DG	N1-C2-N3	-6.48	120.01	123.90	3	10
1	A	2	DC	N3-C2-O2	-6.45	117.39	121.90	6	9
1	A	6	DG	C2-N3-C4	6.43	115.11	111.90	4	6
1	A	6	DG	N1-C2-N3	-6.37	120.08	123.90	4	10
2	B	9	DC	N1-C2-O2	6.35	122.71	118.90	9	9
3	C	18	DG	C2-N3-C4	6.32	115.06	111.90	7	6
3	C	22	DT	P-O5'-C5'	6.31	130.99	120.90	7	1
3	C	21	DC	N1-C2-O2	6.29	122.67	118.90	2	7
1	A	1	DC	N1-C2-O2	6.27	122.66	118.90	8	8
2	B	11	DG	C2-N3-C4	6.23	115.02	111.90	3	6
3	C	16	DC	O4'-C1'-N1	6.21	112.34	108.00	9	1
3	C	25	DG	P-O3'-C3'	6.17	127.10	119.70	1	10
2	B	12	DG	C2-N3-C4	6.09	114.95	111.90	1	6
2	B	8	DA	P-O3'-C3'	6.07	126.98	119.70	1	3
2	B	10	DT	O4'-C1'-N1	6.02	112.21	108.00	2	5
3	C	14	DC	N1-C2-O2	6.00	122.50	118.90	6	7
3	C	15	DC	O4'-C1'-N1	6.00	112.20	108.00	9	2
1	A	2	DC	N3-C4-C5	-6.00	119.50	121.90	3	4
3	C	19	DT	O4'-C1'-N1	5.97	112.18	108.00	3	4
3	C	23	DT	C4'-C3'-C2'	-5.97	97.73	103.10	4	3
3	C	18	DG	N1-C2-N3	-5.96	120.32	123.90	9	3
3	C	20	DA	C1'-O4'-C4'	-5.95	104.15	110.10	1	2
1	A	6	DG	C5-C6-O6	-5.94	125.04	128.60	1	4
2	B	9	DC	C4-C5-C6	5.85	120.32	117.40	9	2
3	C	16	DC	N3-C4-N4	5.73	122.01	118.00	7	2
1	A	5	DA	C5-C6-N6	-5.70	119.14	123.70	8	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	15	DC	N3-C4-N4	5.68	121.98	118.00	7	1
3	C	16	DC	N3-C2-O2	-5.67	117.93	121.90	8	4
3	C	15	DC	C6-N1-C1'	5.66	127.59	120.80	1	5
2	B	12	DG	N1-C2-N3	-5.62	120.53	123.90	9	7
1	A	6	DG	C8-N9-C4	-5.55	104.18	106.40	5	1
2	B	13	DG	C5-C6-O6	-5.51	125.29	128.60	6	1
3	C	20	DA	C8-N9-C4	-5.49	103.60	105.80	7	3
2	B	8	DA	C6-C5-N7	-5.46	128.48	132.30	9	1
3	C	21	DC	N3-C4-C5	-5.35	119.76	121.90	4	2
2	B	12	DG	C5-C6-O6	-5.32	125.41	128.60	9	2
3	C	22	DT	C4-C5-C6	5.31	121.19	118.00	4	1
3	C	23	DT	P-O3'-C3'	5.29	126.04	119.70	1	2
3	C	19	DT	N1-C1'-C2'	5.27	122.62	112.60	7	1
3	C	21	DC	N3-C2-O2	-5.26	118.22	121.90	8	2
3	C	15	DC	N1-C1'-C2'	5.26	122.60	112.60	1	2
3	C	18	DG	N3-C2-N2	5.24	123.57	119.90	1	2
1	A	2	DC	P-O3'-C3'	5.24	125.98	119.70	3	2
3	C	14	DC	C4-C5-C6	5.20	120.00	117.40	5	1
2	B	13	DG	N1-C2-N3	-5.18	120.79	123.90	2	1
2	B	9	DC	C4'-C3'-C2'	-5.17	98.45	103.10	6	3
3	C	26	DG	N1-C2-N3	-5.17	120.80	123.90	1	4
3	C	18	DG	N9-C1'-C2'	5.17	122.42	112.60	8	2
2	B	12	DG	O4'-C1'-N9	-5.13	104.41	108.00	4	3
2	B	13	DG	C2-N3-C4	5.11	114.45	111.90	2	3
3	C	25	DG	N1-C2-N3	-5.09	120.85	123.90	4	3
3	C	16	DC	N3-C4-C5	-5.08	119.87	121.90	6	1
1	A	6	DG	N1-C6-O6	5.06	122.93	119.90	1	2
2	B	9	DC	C2-N1-C1'	5.05	124.35	118.80	2	1
2	B	9	DC	N3-C2-O2	-5.04	118.37	121.90	4	1
3	C	24	DT	C5-C4-O4	5.04	128.43	124.90	8	1
2	B	8	DA	OP1-P-OP2	-5.04	112.05	119.60	3	1

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	B	126	68	68	0±0
3	C	261	149	149	2±1
7	C	98	84	81	0±0
All	All	6170	3710	3669	24

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 2.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:19:DT:C2	7:C:1:BLB:C44	0.54	2.90	5	1
3:C:22:DT:H2'	3:C:23:DT:H72	0.45	1.89	3	8
3:C:18:DG:C5	3:C:19:DT:C4	0.44	3.06	5	1
3:C:23:DT:C2'	3:C:24:DT:H72	0.43	2.44	3	6
3:C:22:DT:C6	3:C:23:DT:H72	0.42	2.50	1	2
2:B:8:DA:C4	2:B:9:DC:C5	0.42	3.07	5	1
3:C:23:DT:C6	3:C:24:DT:H72	0.42	2.50	9	1
3:C:19:DT:H5'	7:C:1:BLB:HAC	0.41	1.91	1	3
7:C:1:BLB:HDC	7:C:1:BLB:C36	0.40	2.46	6	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
8	PEO	C	11	5	1,1,1	0.43±0.03	0±0 (0±0%)
7	BLB	C	1	5	94,103,103	1.18±0.04	9±1 (9±1%)
4	PGA	A	7	-	0,7,8	0.00±0.00	-

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
8	PEO	C	11	5	-	-	-
7	BLB	C	1	5	109,145,145	2.38±0.07	34±2 (31±1%)
4	PGA	A	7	-	0,8,11	0.00±0.00	-

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
7	BLB	C	1	5	-	0±0,88,144,144	0±0,6,6,6
4	PGA	A	7	-	-	0±0,1,5,6	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
7	C	1	BLB	C48-C49	5.23	1.37	1.50	8	10
7	C	1	BLB	O1-C1	4.14	1.16	1.23	3	6
7	C	1	BLB	C42-C43	3.56	1.51	1.49	2	10
7	C	1	BLB	C27-C14	3.50	1.48	1.51	7	10
7	C	1	BLB	C10-C12	3.22	1.45	1.50	2	10
7	C	1	BLB	O58-C58	2.81	1.36	1.43	9	1
7	C	1	BLB	C46-NO	2.73	1.35	1.31	2	10
7	C	1	BLB	C46-C45	2.70	1.40	1.48	4	10
7	C	1	BLB	O40-C40	2.60	1.18	1.23	3	3
7	C	1	BLB	OH1-C14	2.58	1.39	1.44	2	10
7	C	1	BLB	C46-S46	2.53	1.70	1.73	7	10
7	C	1	BLB	O68-C70	2.40	1.30	1.35	1	2
7	C	1	BLB	C4-ND	2.37	1.25	1.32	7	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
7	C	1	BLB	CB-C31-NK	7.84	96.18	109.70	9	10
7	C	1	BLB	C63-OH1-C14	7.83	102.26	114.99	3	10
7	C	1	BLB	O68-C70-NQ	7.32	121.95	110.58	9	7
7	C	1	BLB	O70-C70-NQ	6.07	115.50	125.51	7	10
7	C	1	BLB	C34-C36-NL	6.03	107.30	116.44	4	10
7	C	1	BLB	C5-C6-C7	5.78	120.18	110.64	6	10
7	C	1	BLB	C61-C60-C59	5.72	126.39	113.00	3	10
7	C	1	BLB	CC-C34-C36	5.49	119.81	108.78	4	10
7	C	1	BLB	C14-C13-NH	5.29	115.98	110.20	7	5
7	C	1	BLB	C12-C10-NG	5.17	111.17	115.99	2	10
7	C	1	BLB	O12-C12-C10	4.90	127.92	120.59	6	10
7	C	1	BLB	C50-NP-C49	4.83	133.09	122.08	8	3
7	C	1	BLB	OH1-C14-C27	4.83	118.73	110.59	3	10
7	C	1	BLB	O56-C57-C58	4.57	119.43	107.28	6	10
7	C	1	BLB	O68-C70-O70	4.55	119.09	123.69	7	5
7	C	1	BLB	O62-C60-C59	4.53	117.91	109.69	8	10
7	C	1	BLB	C63-C57-C58	4.52	118.16	110.38	1	9
7	C	1	BLB	OH3-C38-C37	4.48	118.12	109.13	5	10
7	C	1	BLB	OH2-C33-C34	4.28	118.75	108.82	3	10
7	C	1	BLB	C13-NH-C12	4.21	113.92	121.52	8	9
7	C	1	BLB	C33-C34-C36	4.19	102.95	109.37	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
7	C	1	BLB	C45-C44-S43	4.03	106.84	111.79	3	10
7	C	1	BLB	C30-C13-NH	3.85	120.83	110.36	3	10
7	C	1	BLB	C58-C59-C60	3.72	116.88	110.24	4	7
7	C	1	BLB	C13-C30-NK	3.65	108.60	116.48	7	10
7	C	1	BLB	O62-C63-C57	3.56	102.45	109.51	9	10
7	C	1	BLB	C31-NK-C30	3.44	116.76	122.67	1	5
7	C	1	BLB	C64-O56-C57	3.42	109.50	117.96	2	10
7	C	1	BLB	C6-C5-C4	3.22	118.64	112.24	5	1
7	C	1	BLB	CB-C31-C33	3.14	108.63	112.30	7	5
7	C	1	BLB	O36-C36-NL	3.07	128.62	122.93	1	10
7	C	1	BLB	O59-C59-C58	3.06	117.42	110.35	7	1
7	C	1	BLB	C64-O64-C65	3.02	119.62	113.69	6	4
7	C	1	BLB	C5-C4-ND	3.01	108.95	116.21	1	3
7	C	1	BLB	C68-O68-C70	2.98	121.38	117.12	8	8
7	C	1	BLB	CC-C34-C33	2.91	117.23	112.37	9	7
7	C	1	BLB	OH1-C63-C57	2.76	114.70	109.10	9	5
7	C	1	BLB	O68-C68-C67	2.73	113.93	107.70	7	9
7	C	1	BLB	O62-C60-C61	2.69	113.14	106.44	6	1
7	C	1	BLB	C48-C49-NP	2.67	111.84	115.59	8	1
7	C	1	BLB	C51-C50-NP	2.61	104.76	112.21	4	4
7	C	1	BLB	C45-C46-NO	2.52	117.98	124.47	8	1
7	C	1	BLB	C37-NL-C36	2.49	128.24	121.89	9	1
7	C	1	BLB	C59-C58-C57	2.49	115.36	109.68	5	3
7	C	1	BLB	C33-C31-NK	2.44	114.28	109.56	9	2
7	C	1	BLB	O30-C30-NK	2.42	127.42	122.93	6	8
7	C	1	BLB	O58-C58-C57	2.33	116.12	109.94	4	4
7	C	1	BLB	C41-NM-C40	2.26	126.62	122.59	2	5
7	C	1	BLB	OH3-C38-CD	2.24	103.11	109.74	7	1
7	C	1	BLB	O36-C36-C34	2.23	125.04	121.02	4	1
7	C	1	BLB	C9-C10-NG	2.18	120.98	123.31	7	1
7	C	1	BLB	C7-NE-C8	2.18	114.67	118.11	7	1
7	C	1	BLB	C2-C1-NA	2.16	112.98	116.68	6	1
7	C	1	BLB	C3-C2-C1	2.12	112.40	108.66	4	1
7	C	1	BLB	C41-C42-C43	2.11	120.17	112.55	6	1
7	C	1	BLB	O61-C61-C60	2.10	118.48	111.29	3	1
7	C	1	BLB	C9-C10-C12	2.02	127.06	123.14	7	1

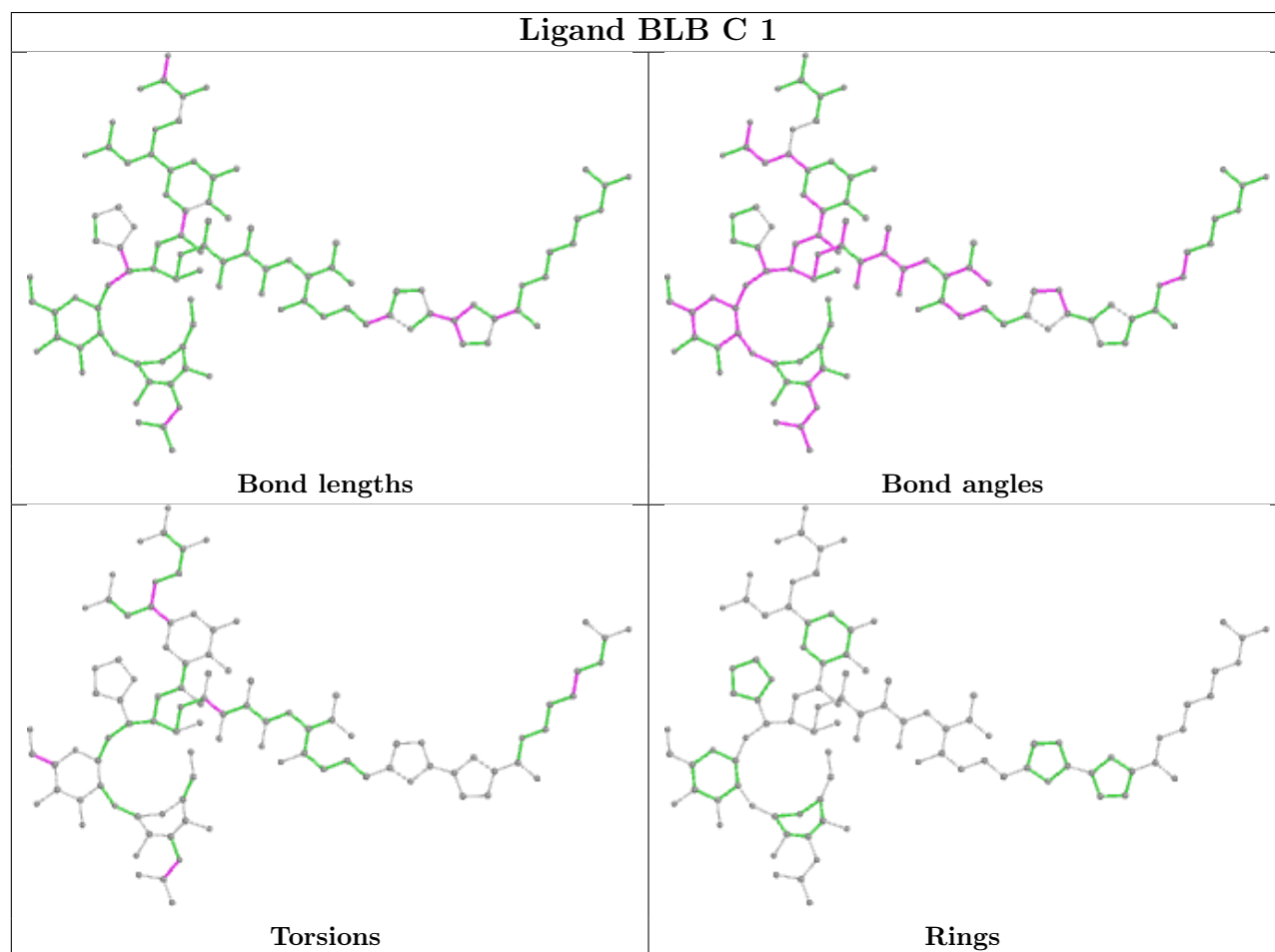
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided