Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 06:16 PM EDT

PDB ID	:	6PFV
Title	:	Structure of S. venezuelae RisG-WhiG-c-di-GMP complex: orthorhombic crystal form
Authors	:	Schumacher, M.A.
Deposited on	:	2019-06-22
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18372 atoms, of which 9070 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein called AmfC protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	T	164	Total	C	H	N	O	S	0	0	0
			2614	788	1306	264	252	4			
1	B	160	Total	C	H	N	O	S	0	0	0
			2514	761	1252	251	246	4			
1	E	159	Total	C	H	N	O	S	0	0	0
			2535	764	1266	256	245	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	24	GLY	-	expression tag	UNP F2RFR7
T	25	SER	-	expression tag	UNP F2RFR7
T	91	GLY	PRO	engineered mutation	UNP F2RFR7
B	24	GLY	-	expression tag	UNP F2RFR7
B	25	SER	-	expression tag	UNP F2RFR7
B	91	GLY	PRO	engineered mutation	UNP F2RFR7
E	24	GLY	-	expression tag	UNP F2RFR7
E	25	SER	-	expression tag	UNP F2RFR7
E	91	GLY	PRO	engineered mutation	UNP F2RFR7

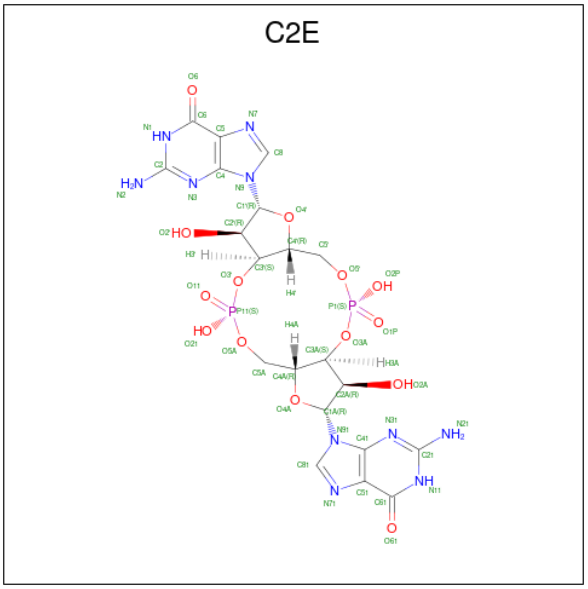
- Molecule 2 is a protein called RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	220	Total	C	H	N	O	S	0	0	0
			3453	1089	1734	299	329	2			
2	D	220	Total	C	H	N	O	S	0	0	0
			3460	1091	1741	299	327	2			
2	G	223	Total	C	H	N	O	S	0	0	0
			3520	1110	1771	307	330	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLU	ASP	engineered mutation	UNP A0A3N1Q704
A	97	VAL	ILE	engineered mutation	UNP A0A3N1Q704
A	144	GLY	ARG	engineered mutation	UNP A0A3N1Q704
A	150	THR	SER	engineered mutation	UNP A0A3N1Q704
A	159	SER	THR	engineered mutation	UNP A0A3N1Q704
A	162	ASP	GLU	engineered mutation	UNP A0A3N1Q704
D	38	GLU	ASP	engineered mutation	UNP A0A3N1Q704
D	97	VAL	ILE	engineered mutation	UNP A0A3N1Q704
D	144	GLY	ARG	engineered mutation	UNP A0A3N1Q704
D	150	THR	SER	engineered mutation	UNP A0A3N1Q704
D	159	SER	THR	engineered mutation	UNP A0A3N1Q704
D	162	ASP	GLU	engineered mutation	UNP A0A3N1Q704
G	38	GLU	ASP	engineered mutation	UNP A0A3N1Q704
G	97	VAL	ILE	engineered mutation	UNP A0A3N1Q704
G	144	GLY	ARG	engineered mutation	UNP A0A3N1Q704
G	150	THR	SER	engineered mutation	UNP A0A3N1Q704
G	159	SER	THR	engineered mutation	UNP A0A3N1Q704
G	162	ASP	GLU	engineered mutation	UNP A0A3N1Q704

- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	T	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	T	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.85Å 97.34Å 204.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.90 – 3.00	Depositor
% Data completeness (in resolution range)	97.0 (87.90-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.214 , 0.278	Depositor
Wilson B-factor (Å^2)	89.1	Xtriage
Anisotropy	0.193	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18372	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

6 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	$\#\|Z\| > 2$
3	C2E	T	201	-	44,52,52	2.08	13 (29%)	52,82,82	1.59	9 (17%)
3	C2E	T	202	-	44,52,52	2.27	15 (34%)	52,82,82	1.56	8 (15%)
3	C2E	E	202	-	44,52,52	2.29	16 (36%)	52,82,82	1.51	7 (13%)
3	C2E	B	201	-	44,52,52	2.39	15 (34%)	52,82,82	1.66	10 (19%)
3	C2E	B	202	-	44,52,52	2.18	15 (34%)	52,82,82	1.67	9 (17%)
3	C2E	E	201	-	44,52,52	2.19	14 (31%)	52,82,82	1.71	9 (17%)

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
3	C2E	T	201	-	-	10/22/62/62	0/6/7/7
3	C2E	T	202	-	-	3/22/62/62	0/6/7/7
3	C2E	E	202	-	-	4/22/62/62	0/6/7/7
3	C2E	B	201	-	-	1/22/62/62	0/6/7/7
3	C2E	B	202	-	-	8/22/62/62	0/6/7/7
3	C2E	E	201	-	-	2/22/62/62	0/6/7/7

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	C2E	C2'-C1'	7.56	1.65	1.53
3	E	202	C2E	C2'-C1'	6.94	1.64	1.53
3	T	202	C2E	C2'-C1'	6.90	1.64	1.53
3	T	201	C2E	C2'-C1'	6.07	1.63	1.53
3	E	201	C2E	C2'-C1'	5.50	1.62	1.53
3	B	202	C2E	C2'-C1'	5.09	1.61	1.53
3	B	202	C2E	C2'-C3'	4.90	1.63	1.52
3	E	201	C2E	C2'-C3'	4.53	1.63	1.52
3	T	202	C2E	P11-O3'	4.46	1.72	1.60
3	E	202	C2E	C2'-C3'	4.43	1.62	1.52
3	T	202	C2E	C2'-C3'	4.40	1.62	1.52
3	E	202	C2E	P11-O3'	4.31	1.71	1.60
3	E	201	C2E	P11-O3'	4.31	1.71	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	C2E	O4'-C1'	4.28	1.47	1.41
3	B	201	C2E	C2'-C3'	4.16	1.62	1.52
3	E	201	C2E	P1-O3A	4.14	1.71	1.60
3	T	201	C2E	C6-N1	4.07	1.43	1.37
3	B	202	C2E	P11-O3'	3.99	1.71	1.60
3	E	201	C2E	O4'-C1'	3.97	1.46	1.41
3	B	201	C2E	P1-O3A	3.93	1.70	1.60
3	B	201	C2E	P11-O3'	3.89	1.70	1.60
3	B	201	C2E	O5'-C5'	-3.77	1.30	1.44
3	E	202	C2E	C61-N11	3.76	1.43	1.37
3	E	202	C2E	O4'-C1'	3.73	1.46	1.41
3	T	202	C2E	C6-N1	3.71	1.43	1.37
3	E	201	C2E	O5'-C5'	-3.69	1.30	1.44
3	T	201	C2E	P11-O3'	3.68	1.70	1.60
3	E	202	C2E	C6-N1	3.67	1.43	1.37
3	B	202	C2E	C6-N1	3.66	1.43	1.37
3	B	201	C2E	C61-N11	3.62	1.43	1.37
3	B	202	C2E	O5'-C5'	-3.59	1.31	1.44
3	B	202	C2E	O4'-C1'	3.53	1.46	1.41
3	T	202	C2E	O5'-C5'	-3.51	1.31	1.44
3	E	201	C2E	C6-N1	3.49	1.43	1.37
3	B	202	C2E	C61-N11	3.49	1.43	1.37
3	B	201	C2E	C6-N1	3.41	1.42	1.37
3	T	202	C2E	C61-N11	3.35	1.42	1.37
3	B	202	C2E	P1-O3A	3.31	1.69	1.60
3	T	202	C2E	O4'-C1'	3.31	1.45	1.41
3	E	202	C2E	P1-O3A	3.20	1.68	1.60
3	T	201	C2E	C2'-C3'	3.14	1.59	1.52
3	T	201	C2E	O4'-C1'	3.10	1.45	1.41
3	T	202	C2E	P1-O3A	3.05	1.68	1.60
3	T	201	C2E	C5-C6	-3.03	1.41	1.47
3	T	201	C2E	P1-O3A	3.02	1.68	1.60
3	E	201	C2E	C61-N11	2.99	1.42	1.37
3	T	201	C2E	C61-N11	2.99	1.42	1.37
3	B	201	C2E	C5-C6	-2.95	1.41	1.47
3	E	202	C2E	O5'-C5'	-2.88	1.33	1.44
3	B	202	C2E	C51-C61	-2.82	1.41	1.47
3	T	202	C2E	C2A-C1A	2.80	1.58	1.53
3	B	202	C2E	C5-C6	-2.80	1.41	1.47
3	T	202	C2E	C51-C61	-2.80	1.41	1.47
3	E	201	C2E	C51-C61	-2.79	1.41	1.47
3	T	202	C2E	C5-C6	-2.79	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	C2E	C2A-C1A	2.79	1.58	1.53
3	E	202	C2E	C5-C6	-2.78	1.41	1.47
3	B	201	C2E	C51-C61	-2.77	1.41	1.47
3	T	201	C2E	O4A-C1A	-2.72	1.37	1.41
3	E	202	C2E	C51-C61	-2.71	1.41	1.47
3	E	201	C2E	O2A-C2A	-2.69	1.36	1.43
3	B	202	C2E	O2A-C2A	-2.67	1.36	1.43
3	E	201	C2E	P11-O5A	2.60	1.69	1.59
3	B	201	C2E	P11-O5A	2.56	1.69	1.59
3	E	201	C2E	C5-C6	-2.52	1.42	1.47
3	B	201	C2E	C5A-C4A	2.52	1.59	1.51
3	B	202	C2E	C2A-C1A	2.51	1.57	1.53
3	T	202	C2E	O2A-C2A	-2.50	1.37	1.43
3	B	201	C2E	O2A-C2A	-2.49	1.37	1.43
3	E	202	C2E	O2A-C2A	-2.48	1.37	1.43
3	B	202	C2E	P11-O5A	2.46	1.69	1.59
3	E	202	C2E	P1-O5'	2.44	1.69	1.59
3	T	201	C2E	O3'-C3'	-2.42	1.35	1.44
3	E	202	C2E	P11-O5A	2.39	1.69	1.59
3	T	201	C2E	O2A-C2A	-2.32	1.37	1.43
3	B	202	C2E	C5A-C4A	2.23	1.58	1.51
3	T	202	C2E	O3A-C3A	-2.22	1.36	1.44
3	E	201	C2E	C5A-C4A	2.18	1.58	1.51
3	T	202	C2E	P11-O5A	2.18	1.68	1.59
3	B	202	C2E	O3A-C3A	-2.17	1.36	1.44
3	T	201	C2E	P1-O5'	2.17	1.68	1.59
3	T	202	C2E	C8-N7	-2.16	1.31	1.35
3	B	201	C2E	P1-O5'	2.11	1.67	1.59
3	E	202	C2E	C2A-C1A	2.09	1.56	1.53
3	E	202	C2E	C5A-C4A	2.04	1.58	1.51
3	T	201	C2E	O5'-C5'	-2.04	1.36	1.44
3	E	202	C2E	C21-N21	2.03	1.39	1.34
3	E	201	C2E	C2A-C1A	2.02	1.56	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	C2E	O6-C6-C5	4.17	132.51	124.37
3	T	202	C2E	O6-C6-C5	4.10	132.39	124.37
3	E	201	C2E	O6-C6-C5	4.10	132.38	124.37
3	T	201	C2E	O61-C61-N11	-4.06	115.86	120.65
3	E	202	C2E	O6-C6-C5	4.01	132.19	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	201	C2E	O61-C61-C51	3.93	132.05	124.37
3	B	201	C2E	O6-C6-C5	3.85	131.90	124.37
3	E	201	C2E	O61-C61-C51	3.75	131.70	124.37
3	E	201	C2E	O6-C6-N1	-3.67	116.31	120.65
3	B	202	C2E	O6-C6-N1	-3.63	116.37	120.65
3	B	202	C2E	O61-C61-C51	3.60	131.41	124.37
3	B	201	C2E	O61-C61-C51	3.59	131.38	124.37
3	T	202	C2E	O61-C61-C51	3.55	131.31	124.37
3	B	202	C2E	O61-C61-N11	-3.47	116.55	120.65
3	E	202	C2E	O6-C6-N1	-3.47	116.56	120.65
3	B	202	C2E	O21-P11-O11	3.42	129.16	112.24
3	T	201	C2E	O21-P11-O11	3.41	129.11	112.24
3	B	201	C2E	O61-C61-N11	-3.41	116.63	120.65
3	T	201	C2E	O6-C6-C5	3.40	131.00	124.37
3	T	202	C2E	O6-C6-N1	-3.39	116.64	120.65
3	T	202	C2E	O61-C61-N11	-3.37	116.67	120.65
3	E	202	C2E	O61-C61-C51	3.36	130.93	124.37
3	B	201	C2E	O2P-P1-O1P	3.34	128.77	112.24
3	E	201	C2E	O2P-P1-O1P	3.32	128.68	112.24
3	B	201	C2E	C2'-C3'-C4'	3.31	109.09	103.22
3	E	201	C2E	C5'-C4'-C3'	-3.31	103.45	114.40
3	B	201	C2E	O21-P11-O11	3.26	128.34	112.24
3	T	202	C2E	O21-P11-O11	3.24	128.26	112.24
3	E	201	C2E	C2'-C3'-C4'	3.24	108.96	103.22
3	E	201	C2E	O61-C61-N11	-3.21	116.86	120.65
3	B	202	C2E	O2P-P1-O1P	3.20	128.08	112.24
3	T	202	C2E	O2P-P1-O1P	3.18	127.98	112.24
3	T	201	C2E	O2P-P1-O1P	3.16	127.85	112.24
3	B	201	C2E	O6-C6-N1	-3.15	116.92	120.65
3	E	202	C2E	O21-P11-O11	3.15	127.81	112.24
3	E	202	C2E	O2P-P1-O1P	3.15	127.81	112.24
3	E	201	C2E	O21-P11-O11	3.12	127.66	112.24
3	B	202	C2E	C5'-C4'-C3'	-3.09	104.15	114.40
3	B	201	C2E	C5'-C4'-C3'	-3.06	104.26	114.40
3	E	202	C2E	O61-C61-N11	-3.01	117.09	120.65
3	B	202	C2E	C2'-C3'-C4'	2.62	107.87	103.22
3	T	201	C2E	O6-C6-N1	-2.55	117.64	120.65
3	T	202	C2E	C5'-C4'-C3'	-2.30	106.78	114.40
3	T	201	C2E	O4A-C4A-C3A	2.23	109.64	104.87
3	E	202	C2E	C2'-C3'-C4'	2.16	107.06	103.22
3	T	201	C2E	O4'-C1'-C2'	2.16	110.08	106.93
3	B	201	C2E	N1-C2-N3	2.12	127.28	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	C2E	N1-C2-N3	2.05	127.15	123.32
3	B	201	C2E	O4A-C4A-C3A	2.05	109.25	104.87
3	T	202	C2E	N1-C2-N3	2.04	127.13	123.32
3	T	201	C2E	N1-C2-N3	2.01	127.08	123.32
3	E	201	C2E	N1-C2-N3	2.01	127.07	123.32

There are no chirality outliers.

All (28) torsion outliers are listed below:

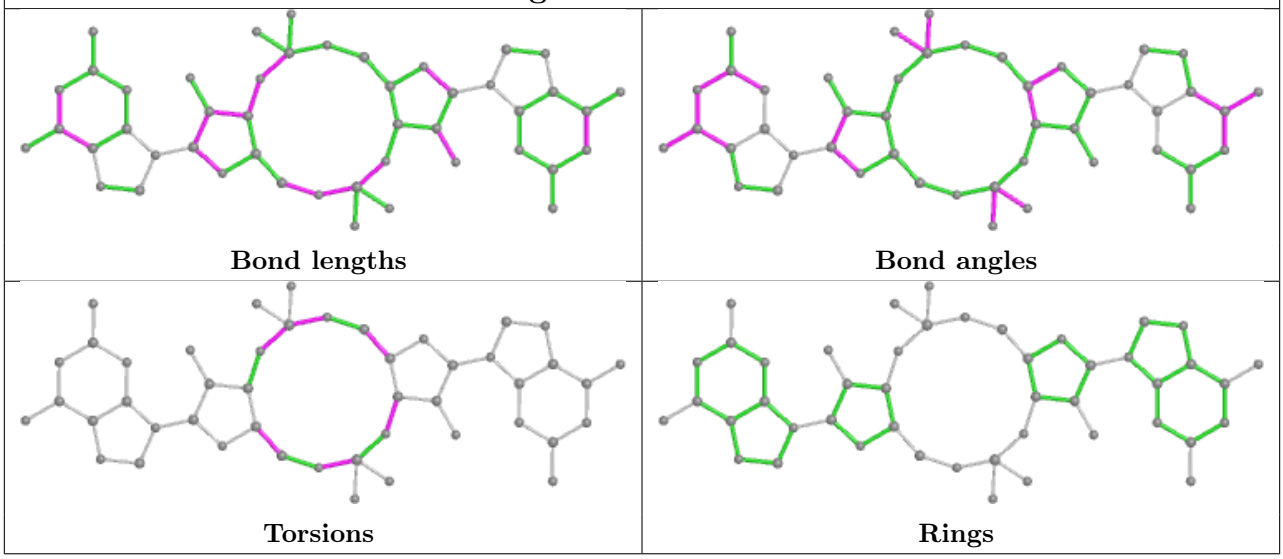
Mol	Chain	Res	Type	Atoms
3	T	201	C2E	C3'-O3'-P11-O5A
3	T	201	C2E	O4A-C4A-C5A-O5A
3	B	202	C2E	C5A-O5A-P11-O21
3	E	201	C2E	C3'-O3'-P11-O5A
3	E	201	C2E	C5A-O5A-P11-O21
3	T	201	C2E	O4'-C4'-C5'-O5'
3	T	201	C2E	C3'-C4'-C5'-O5'
3	T	202	C2E	C3'-C4'-C5'-O5'
3	T	201	C2E	C3A-C4A-C5A-O5A
3	T	201	C2E	C5'-O5'-P1-O3A
3	T	201	C2E	C5A-O5A-P11-O3'
3	B	202	C2E	C5A-O5A-P11-O3'
3	E	202	C2E	O4A-C4A-C5A-O5A
3	T	202	C2E	O4'-C4'-C5'-O5'
3	T	202	C2E	C3'-O3'-P11-O5A
3	B	201	C2E	C3'-O3'-P11-O5A
3	E	202	C2E	C3A-C4A-C5A-O5A
3	B	202	C2E	C3'-O3'-P11-O5A
3	E	202	C2E	C3'-O3'-P11-O5A
3	B	202	C2E	O4A-C4A-C5A-O5A
3	T	201	C2E	C5'-O5'-P1-O1P
3	T	201	C2E	C5A-O5A-P11-O11
3	B	202	C2E	C5A-O5A-P11-O11
3	B	202	C2E	C3'-C4'-C5'-O5'
3	E	202	C2E	C3'-C4'-C5'-O5'
3	B	202	C2E	C3A-O3A-P1-O5'
3	B	202	C2E	O4'-C4'-C5'-O5'
3	T	201	C2E	C4A-C3A-O3A-P1

There are no ring outliers.

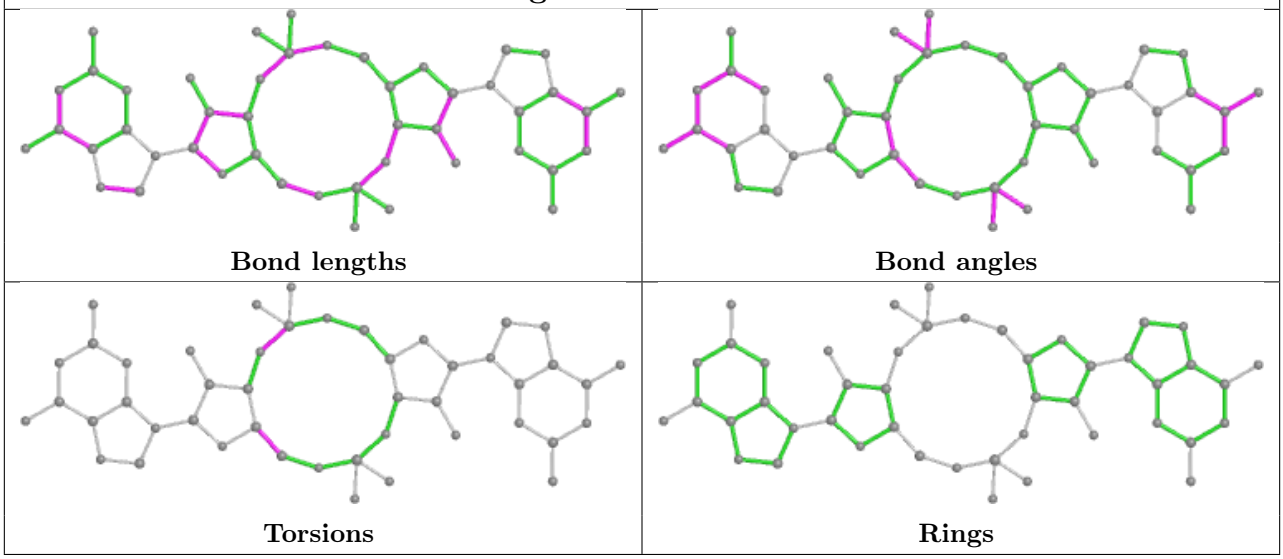
No monomer is involved in short contacts.

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.

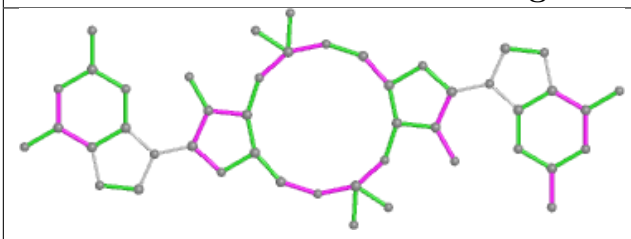
Ligand C2E T 201



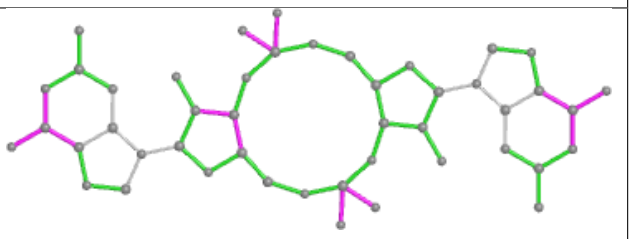
Ligand C2E T 202



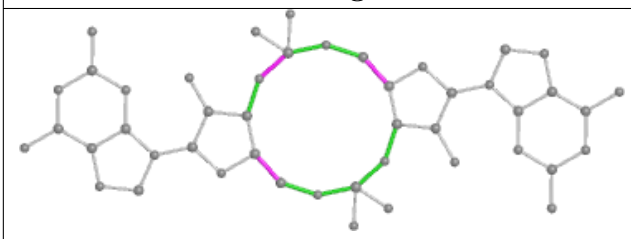
Ligand C2E E 202



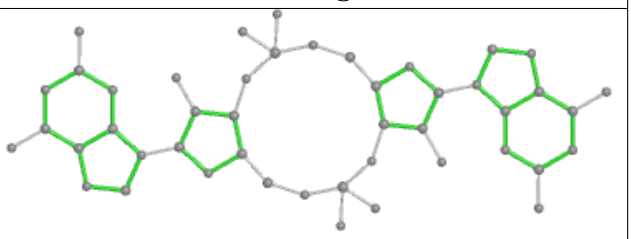
Bond lengths



Bond angles

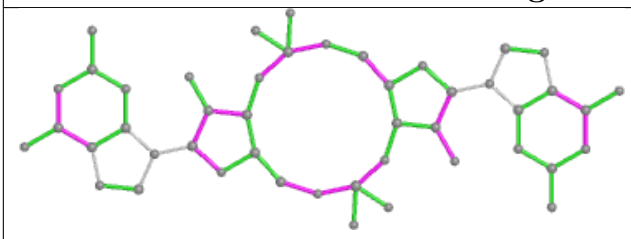


Torsions

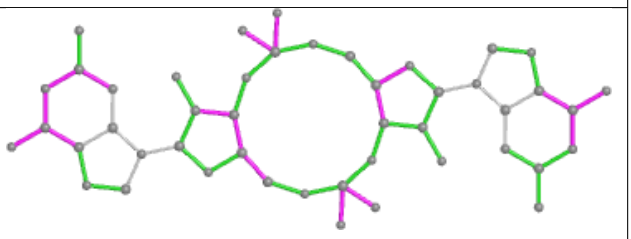


Rings

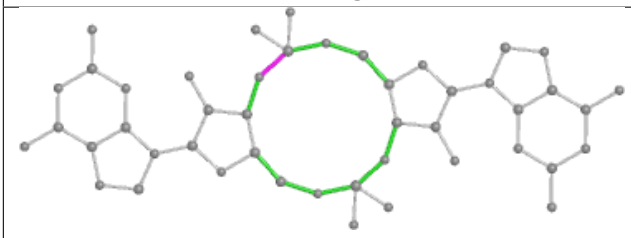
Ligand C2E B 201



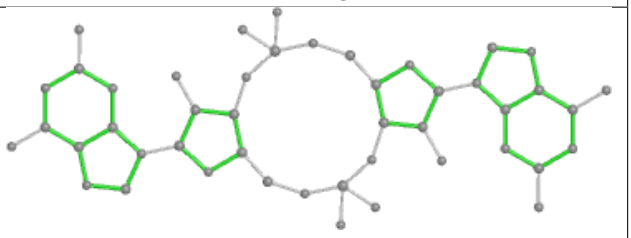
Bond lengths



Bond angles

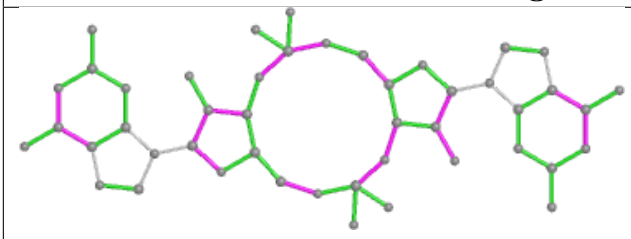


Torsions

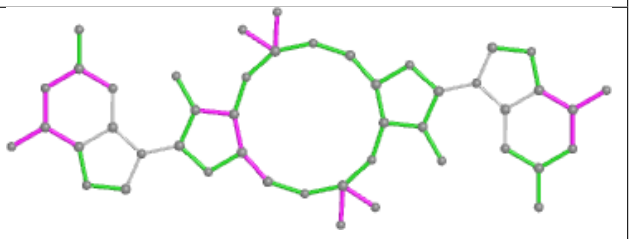


Rings

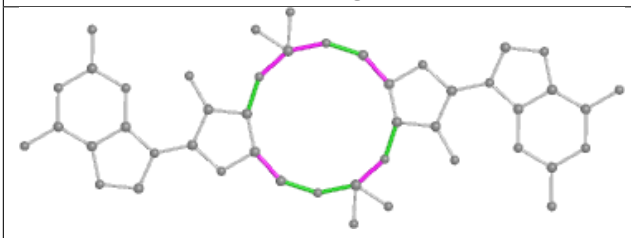
Ligand C2E B 202



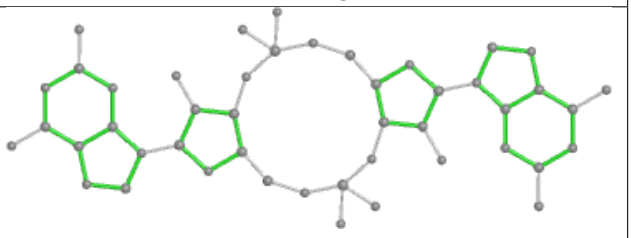
Bond lengths



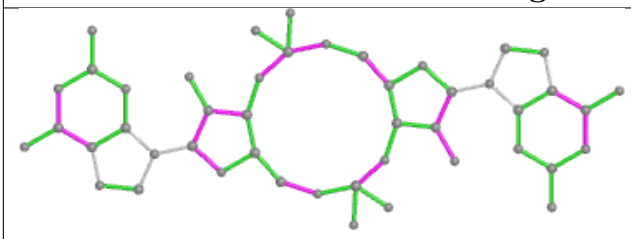
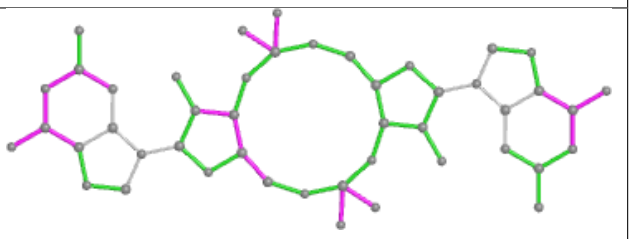
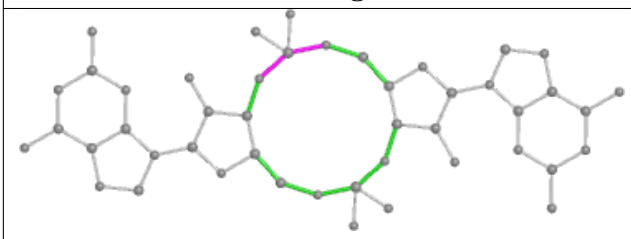
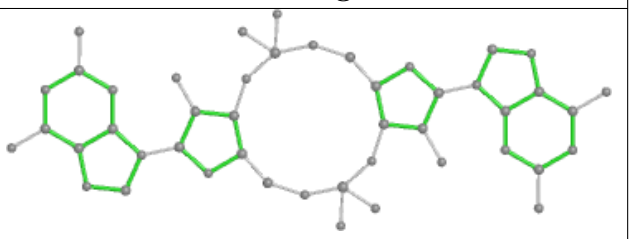
Bond angles



Torsions



Rings

Ligand C2E E 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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