

wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 03:36 PM EST

PDB ID : 128D

Title: MOLECULAR STRUCTURE OF D(CGC[E6G]AATTCGCG) COM-

PLEXED WITH HOECHST 33258

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Deposited on : 1993-06-30

Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

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)

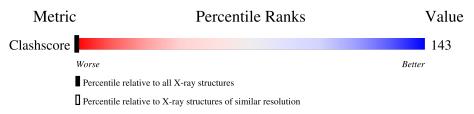
Validation Pipeline (wwPDB-VP) : 2.36

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 2.50 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\#\text{Entries, resolution range}(\text{\AA}))$
Clashscore	141614	5346 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	A	12	8% 92%					
1	В	12	100%					

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HT	A	25	-	-	X	-



2 Entry composition (i)

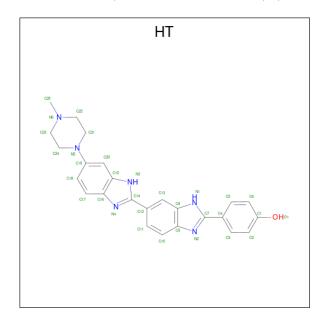
There are 3 unique types of molecules in this entry. The entry contains 590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA chain called DNA (5'-D(*CP*GP*CP*(G36)P*AP*AP*TP*TP*CP* GP*CP*G)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	12	Total	С	N	О	Р	0	0	0
1	A	12	245	118	46	70	11	0	U	U
1	D	12	Total	С	N	О	Р	0	0	0
1	Б	12	245	118	46	70	11	0	U	U

• Molecule 2 is 2'-(4-HYDROXYPHENYL)-5-(4-METHYL-1-PIPERAZINYL)-2,5'-BI-BENZ IMIDAZOLE (three-letter code: HT) (formula: $C_{25}H_{24}N_6O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 32	C 25	N 6	O 1	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	В	49	Total O 49 49	0	0



3 Residue-property plots (i)

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.

Note EDS was not executed.

C13 G16 G16 G16 G16 G26 G27 G22 G22

Note EDS was not e	xecuted.	
• Molecule 1: DNA	(5'-D(*CP*GP*CP*(G36)P*AP*AP*TP*TP*CP*GP*(CP*G)-3')
Chain A: 8%	92%	
C1 G2 C3 G4 A6 A6 T7 T7 T78 C10 C11		
• Molecule 1: DNA	(5'-D(*CP*GP*CP*(G36)P*AP*AP*TP*TP*CP*GP*	CP*G)-3')
Chain B:	100%	



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	25.64Å 41.31 Å 66.99 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) - 2.50	Depositor
% Data completeness	(Not available) ((Not available)-2.50)	Depositor
(in resolution range)		Беровног
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	NUCLSQ	Depositor
R, R_{free}	0.145 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	590	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP



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: G36, HT

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	2.40	13/246 (5.3%)	3.47	55/375 (14.7%)	
1	В	2.29	$11/246 \ (4.5\%)$	3.73	61/375 (16.3%)	
All	All	2.34	$24/492 \ (4.9\%)$	3.61	116/750 (15.5%)	

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	9	DC	P-O5'	8.57	1.68	1.59
1	A	12	DG	P-O5'	-7.45	1.52	1.59
1	В	13	DC	O3'-P	-7.36	1.52	1.61
1	A	6	DA	O3'-P	7.33	1.70	1.61
1	A	11	DC	P-OP2	6.43	1.59	1.49

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	В	13	DC	P-O3'-C3'	17.90	141.18	119.70
1	A	3	DC	O4'-C1'-N1	14.82	118.37	108.00
1	В	14	DG	O4'-C1'-N9	14.40	118.08	108.00
1	В	19	DT	O4'-C4'-C3'	-12.03	98.78	106.00
1	В	19	DT	O4'-C1'-N1	11.23	115.86	108.00

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	245	0	140	65	2
1	В	245	0	140	59	0
2	A	32	0	23	17	0
3	A	19	0	0	0	0
3	В	49	0	0	0	0
All	All	590	0	303	118	2

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 143.

The worst 5 of 118 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
2:A:25:HT:H231	1:B:17:DA:C2	1.87	1.09	
1:A:6:DA:H1'	1:A:7:DT:H5'	1.25	1.09	
1:A:9:DC:O2	2:A:25:HT:H232	1.58	1.04	
1:A:9:DC:O4'	2:A:25:HT:H241	1.57	1.02	
1:B:18:DA:H2'	1:B:19:DT:H71	1.47	0.97	

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:A:1:DC:O5'	1:A:7:DT:OP2[3_655]	2.05	0.15	
1:A:1:DC:C5'	1:A:7:DT:OP2[3_655]	2.08	0.12	

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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		Ros	Res	Ros	Link	Bo	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	Lilik		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
1	G36	A	4	1	20,26,27	1.45	3 (15%)	21,37,40	3.90	5 (23%)		
1	G36	В	16	1	20,26,27	1.42	3 (15%)	21,37,40	2.25	8 (38%)		

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	G36	A	4	1	-	4/6/24/25	0/3/3/3
1	G36	В	16	1	-	5/6/24/25	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}({ ext{ iny A}})$
1	A	4	G36	C6-N1	3.56	1.37	1.31
1	В	16	G36	C6-N1	3.03	1.36	1.31
1	A	4	G36	O4'-C1'	2.81	1.48	1.42
1	A	4	G36	O6-C1M	-2.80	1.33	1.43
1	В	16	G36	O4'-C4'	-2.19	1.40	1.45

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	A	4	G36	C1M-O6-C6	14.27	131.66	117.56

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	4	G36	O6-C6-N1	-7.37	113.77	120.12
1	A	4	G36	C5-C6-N1	-4.57	114.55	123.26
1	В	16	G36	C5-C6-N1	-4.52	114.65	123.26
1	В	16	G36	C1M-O6-C6	4.09	121.60	117.56

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	4	G36	C5-C6-O6-C1M
1	A	4	G36	N1-C6-O6-C1M
1	A	4	G36	CM2-C1M-O6-C6
1	В	16	G36	O4'-C4'-C5'-O5'
1	В	16	G36	C5-C6-O6-C1M

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4	G36	3	0
1	В	16	G36	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 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	Chain	Chain	Chain	Res	Link	B	ond leng	gths	В	ond ang	gles
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2			
2	HT	A	25	-	35,37,37	2.60	16 (45%)	32,54,54	2.84	11 (34%)			



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
2	НТ	A	25	-	-	2/4/22/22	0/6/6/6

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
2	A	25	HT	C7-N1	5.36	1.44	1.34
2	A	25	HT	O1-C1	-4.79	1.25	1.37
2	A	25	HT	C20-C15	-4.30	1.35	1.41
2	A	25	HT	C14-N3	4.14	1.42	1.34
2	A	25	HT	C17-C18	3.92	1.44	1.36

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	A	25	HT	C23-N6-C22	9.06	122.19	109.52
2	A	25	HT	C24-C23-N6	4.98	116.43	110.80
2	A	25	HT	C22-C21-N5	4.92	120.26	110.70
2	A	25	HT	C24-N5-C21	4.34	121.10	111.52
2	A	25	HT	C20-C19-N5	-4.18	116.93	121.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	25	HT	C20-C19-N5-C21
2	A	25	HT	C18-C19-N5-C21

There are no ring outliers.

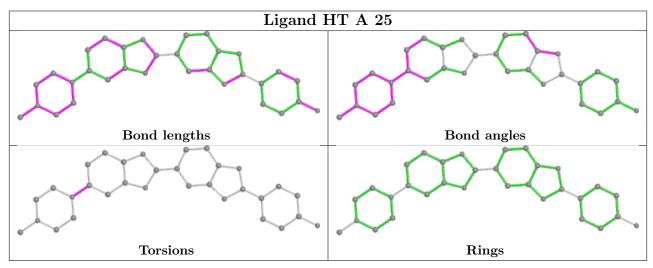
1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	25	HT	17	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 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.



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.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

