



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2025 – 10:07 am BST

PDB ID : 9FTA / pdb\_00009fta  
Title : Crystal structure of d(GGGGTTTTGGGG) with Zn and K  
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Deposited on : 2024-06-24  
Resolution : 2.49 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : **FAILED**  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

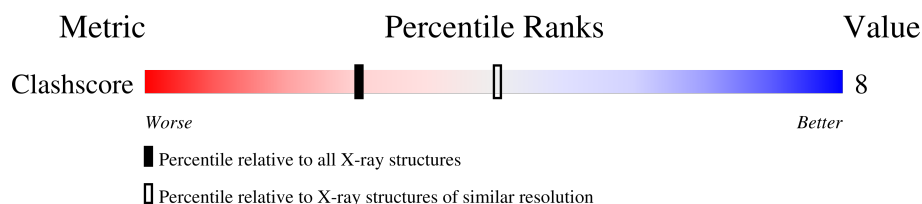
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	6282 (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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain	
1	AAA	12		75%      25%
1	BBB	12		58%      42%
1	CCC	12		67%      33%
1	DDD	12		75%      25%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1070 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(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	BBB	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	CCC	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	DDD	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	6	Total	K	0	0
			6	6		
2	BBB	1	Total	K	0	0
			1	1		
2	CCC	5	Total	K	0	0
			5	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Zn	0	0
			1	1		
3	BBB	2	Total	Zn	0	0
			2	2		
3	DDD	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest"

by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	DDD	1	Total 1	Na 1	0	0

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	10	Total 10	O 10	0	0
5	BBB	11	Total 11	O 11	0	0
5	CCC	11	Total 11	O 11	0	0
5	DDD	9	Total 9	O 9	0	0

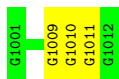
### 3 Residue-property plots [i](#)

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 failed to run properly.

- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*GP\*G)-3')

Chain AAA: 



- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*GP\*G)-3')

Chain BBB: 




- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*GP\*G)-3')

Chain CCC: 



- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*GP\*G)-3')

Chain DDD: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	26.46Å 47.92Å 96.08Å 90.00° 89.92° 90.06°	Depositor
Resolution (Å)	48.04 – 2.49	Depositor
% Data completeness (in resolution range)	91.1 (48.04-2.49)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.334 , 0.426	Depositor
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.135	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3899e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: K, NA, ZN

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	AAA	0.36	0/284	0.82	0/440
1	BBB	0.37	0/284	0.83	0/440
1	CCC	0.36	0/284	0.90	1/440 (0.2%)
1	DDD	0.40	0/284	0.77	0/440
All	All	0.37	0/1136	0.83	1/1760 (0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	1010	DG	C2'-C3'-O3'	6.15	120.73	111.50

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	AAA	253	0	138	2	0
1	BBB	253	0	138	4	0
1	CCC	253	0	138	3	0
1	DDD	253	0	138	2	0
2	AAA	6	0	0	0	0
2	BBB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	5	0	0	0	0
3	AAA	1	0	0	0	0
3	BBB	2	0	0	0	0
3	DDD	1	0	0	0	0
4	DDD	1	0	0	0	0
5	AAA	10	0	0	0	0
5	BBB	11	0	0	1	0
5	CCC	11	0	0	0	0
5	DDD	9	0	0	0	0
All	All	1070	0	552	9	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 8.

The worst 5 of 9 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:BBB:2010:DG:H3'	5:BBB:2201:HOH:O	2.06	0.54
1:AAA:1009:DG:OP1	1:DDD:2012:DG:O3'	2.23	0.51
1:BBB:2006:DT:H2''	1:BBB:2008:DT:O4	2.13	0.49
1:DDD:2006:DT:H2''	1:DDD:2008:DT:O4	2.13	0.49
1:AAA:1010:DG:H2''	1:AAA:1011:DG:OP2	2.13	0.48

There are no symmetry-related clashes.

## 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](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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