



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:08 pm BST

PDB ID : 244D
Title : THE HIGH-RESOLUTION CRYSTAL STRUCTURE OF A PARALLEL-STRANDED GUANINE TETRAPLEX
Authors : Laughlan, G.; Murchie, A.I.H.; Norman, D.G.; Moore, M.H.; Moody, P.C.E.; Lilley, D.M.J.; Luisi, B.
Deposited on : 1995-10-19
Resolution : 1.20 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.11

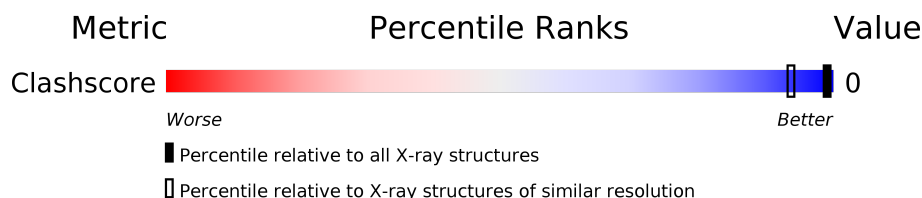
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 Å.

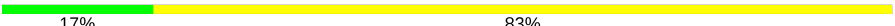
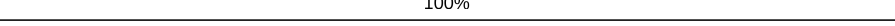
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1286 (1.22-1.18)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	6	 100%
1	B	6	 17% 83%
1	C	6	 17% 83%
1	D	6	 100%
1	E	6	 100%
1	F	6	 100%
1	G	6	 100%
1	H	6	 100%
1	I	6	 33% 67%
1	J	6	 83% 17%

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Mol	Chain	Length	Quality of chain
1	K	6	 17%83%
1	L	6	 100%
1	M	6	 100%
1	N	6	 17%83%
1	O	6	 100%
1	P	6	 17%67%17%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2453 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(*TP*GP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	B	6	Total	C	N	O	P	0	0	0
			108	50	22	31	5			
1	C	6	Total	C	N	O	P	0	0	1
			109	50	22	32	5			
1	D	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	E	6	Total	C	N	O	P	0	0	0
			108	50	22	31	5			
1	F	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	G	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	H	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	I	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	J	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	K	6	Total	C	N	O	P	0	0	0
			108	50	22	31	5			
1	L	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	M	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	N	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			
1	O	6	Total	C	N	O	P	0	0	0
			108	50	22	31	5			
1	P	6	Total	C	N	O	P	0	0	0
			125	60	24	36	5			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	3	Total 3	Na 3	0	0
2	B	1	Total 1	Na 1	0	0
2	I	3	Total 3	Na 3	0	0
2	A	3	Total 3	Na 3	0	0
2	L	1	Total 1	Na 1	0	0
2	M	3	Total 3	Na 3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	2	Total 2	Ca 2	0	0
3	N	1	Total 1	Ca 1	0	0
3	L	1	Total 1	Ca 1	0	0
3	M	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total 37	O 37	0	0
4	B	32	Total 32	O 32	0	0
4	C	26	Total 26	O 26	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	49	Total 49	O 49	0	0
4	E	28	Total 28	O 28	0	0
4	F	28	Total 28	O 28	0	0
4	G	31	Total 31	O 31	0	0
4	H	28	Total 28	O 28	0	0
4	I	36	Total 36	O 36	0	0
4	J	24	Total 24	O 24	0	0
4	K	19	Total 19	O 19	0	0
4	L	37	Total 37	O 37	0	0
4	M	41	Total 41	O 41	0	0
4	N	35	Total 35	O 35	0	0
4	O	28	Total 28	O 28	0	0
4	P	35	Total 35	O 35	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain A:  100%

T1
G2
G3
G4
G5
T6

- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain B:  17% 83%

T11
G12
G13
G14
G15
T16

- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain C:  17% 83%

T21
G22
G23
G24
G25
T26

- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain D:  100%

T31
G32
G33
G34
G35
T36

- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain E:  100%

T41
G42
G43
G44
G45
T46

- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain F:  100%

T51
G52
G53
G54
G55
T56

- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')



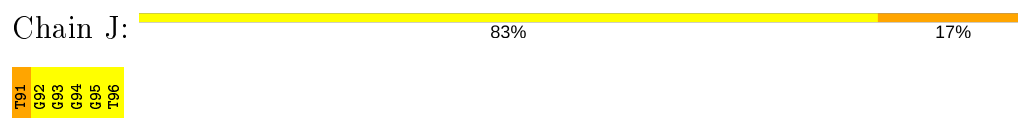
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')



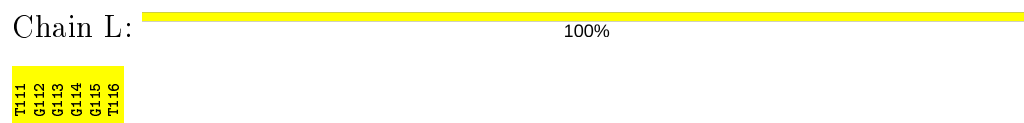
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

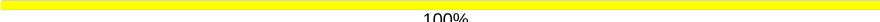


- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')



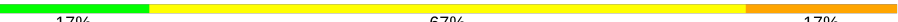
T131	G132	G133	G134	G135	T136
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- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain O:  100%

T141	G142	G143	G144	G145	T146
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- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain P:  17% 67% 17%

T151	G152	G153	G154	G155	T156
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	28.76 Å 35.47 Å 56.77 Å 74.39° 77.64° 89.73°	Depositor
Resolution (Å)	8.00 – 1.20	Depositor
% Data completeness (in resolution range)	97.7 (8.00-1.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELX-93	Depositor
R, R_{free}	0.124 , 0.176	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2453	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA

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	A	2.06	4/140 (2.9%)	2.69	14/216 (6.5%)
1	B	1.82	0/121	2.92	9/186 (4.8%)
1	C	2.06	3/122 (2.5%)	2.61	11/189 (5.8%)
1	D	2.03	6/140 (4.3%)	2.51	16/216 (7.4%)
1	E	1.91	2/121 (1.7%)	2.57	6/186 (3.2%)
1	F	2.21	7/140 (5.0%)	2.83	21/216 (9.7%)
1	G	2.15	4/140 (2.9%)	2.92	19/216 (8.8%)
1	H	1.95	2/140 (1.4%)	2.67	18/216 (8.3%)
1	I	2.19	4/140 (2.9%)	2.48	11/216 (5.1%)
1	J	1.84	2/140 (1.4%)	2.86	21/216 (9.7%)
1	K	2.02	3/121 (2.5%)	3.22	16/186 (8.6%)
1	L	2.26	5/140 (3.6%)	2.88	15/216 (6.9%)
1	M	2.02	6/140 (4.3%)	2.42	15/216 (6.9%)
1	N	2.19	3/140 (2.1%)	3.26	18/216 (8.3%)
1	O	2.19	5/121 (4.1%)	2.69	12/186 (6.5%)
1	P	1.93	2/140 (1.4%)	3.09	20/216 (9.3%)
All	All	2.06	58/2146 (2.7%)	2.80	242/3309 (7.3%)

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	81	DT	C5-C7	10.38	1.56	1.50
1	F	51	DT	C5-C7	8.78	1.55	1.50
1	M	122	DG	C2'-C1'	8.08	1.60	1.52
1	L	111	DT	C5-C7	7.81	1.54	1.50
1	G	66	DT	O4'-C1'	7.27	1.50	1.42

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	131	DT	P-O3'-C3'	24.31	148.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	DT	OP1-P-OP2	21.63	152.05	119.60
1	K	106	DT	OP1-P-OP2	-19.06	91.01	119.60
1	E	46	DT	OP1-P-OP2	17.50	145.85	119.60
1	K	102	DG	OP1-P-OP2	15.91	143.46	119.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A	125	0	70	0	0
1	B	108	0	57	0	0
1	C	109	0	57	0	0
1	D	125	0	70	0	0
1	E	108	0	57	0	0
1	F	125	0	70	0	0
1	G	125	0	69	0	0
1	H	125	0	70	0	0
1	I	125	0	70	0	0
1	J	125	0	70	1	0
1	K	108	0	57	0	0
1	L	125	0	70	0	0
1	M	125	0	70	0	0
1	N	125	0	70	0	0
1	O	108	0	57	0	0
1	P	125	0	70	1	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	E	3	0	0	0	0
2	I	3	0	0	0	0
2	L	1	0	0	0	0
2	M	3	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	P	1	0	0	0	0
4	A	37	0	0	0	0
4	B	32	0	0	0	0
4	C	26	0	0	0	0
4	D	49	0	0	0	0
4	E	28	0	0	0	0
4	F	28	0	0	0	0
4	G	31	0	0	0	0
4	H	28	0	0	0	0
4	I	36	0	0	0	0
4	J	24	0	0	0	0
4	K	19	0	0	0	0
4	L	37	0	0	0	0
4	M	41	0	0	0	0
4	N	35	0	0	0	0
4	O	28	0	0	0	0
4	P	35	0	0	0	0
All	All	2453	0	1054	1	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 0.

All (1) 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:J:91:DT:O4'	1:P:151:DT:H2'	2.19	0.42

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 23 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.