



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 04:38 PM GMT

PDB ID : 2G4C  
Title : Crystal Structure of human DNA polymerase gamma accessory subunit  
Authors : Fan, L.; Farr, C.L.; Kaguni, L.S.; Tainer, J.A.  
Deposited on : 2006-02-22  
Resolution : 3.15 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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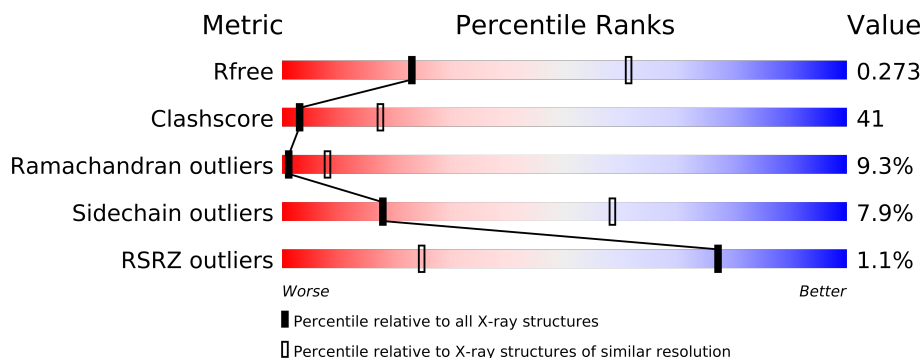
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.15 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))
$R_{free}$	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	474	
1	B	474	
1	C	474	
1	D	474	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12847 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA polymerase gamma subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3202	2050	558	578	16			
1	B	397	Total	C	N	O	S	0	0	0
			3202	2050	558	578	16			
1	C	397	Total	C	N	O	S	0	0	0
			3206	2053	560	577	16			
1	D	397	Total	C	N	O	S	0	0	0
			3206	2053	560	577	16			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	INITIATING METHIONINE	UNP Q9UHN1
A	13	ARG	-	CLONING ARTIFACT	UNP Q9UHN1
A	14	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
A	15	SER	-	CLONING ARTIFACT	UNP Q9UHN1
A	16	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	17	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	18	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	19	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	20	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	21	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	22	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
A	23	SER	-	CLONING ARTIFACT	UNP Q9UHN1
A	24	THR	-	CLONING ARTIFACT	UNP Q9UHN1
A	25	MET	-	CLONING ARTIFACT	UNP Q9UHN1
A	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
B	12	MET	-	INITIATING METHIONINE	UNP Q9UHN1
B	13	ARG	-	CLONING ARTIFACT	UNP Q9UHN1
B	14	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
B	15	SER	-	CLONING ARTIFACT	UNP Q9UHN1
B	16	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	17	HIS	-	EXPRESSION TAG	UNP Q9UHN1

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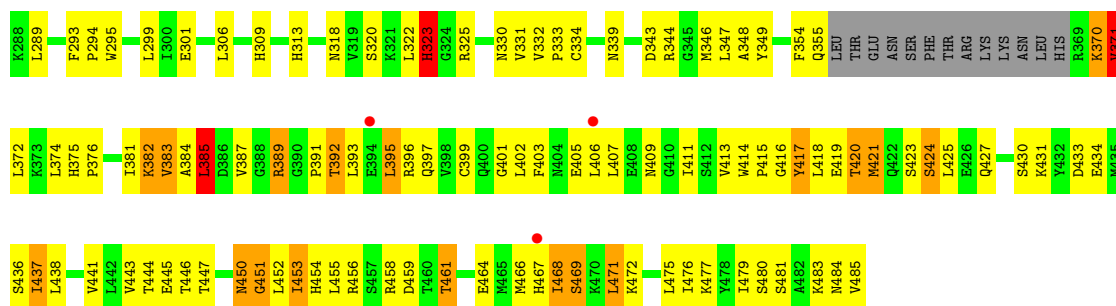
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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	19	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	20	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	21	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	22	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
B	23	SER	-	CLONING ARTIFACT	UNP Q9UHN1
B	24	THR	-	CLONING ARTIFACT	UNP Q9UHN1
B	25	MET	-	CLONING ARTIFACT	UNP Q9UHN1
B	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
C	12	MET	-	INITIATING METHIONINE	UNP Q9UHN1
C	13	ARG	-	CLONING ARTIFACT	UNP Q9UHN1
C	14	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
C	15	SER	-	CLONING ARTIFACT	UNP Q9UHN1
C	16	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	17	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	18	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	19	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	20	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	21	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	22	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
C	23	SER	-	CLONING ARTIFACT	UNP Q9UHN1
C	24	THR	-	CLONING ARTIFACT	UNP Q9UHN1
C	25	MET	-	CLONING ARTIFACT	UNP Q9UHN1
C	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
D	12	MET	-	INITIATING METHIONINE	UNP Q9UHN1
D	13	ARG	-	CLONING ARTIFACT	UNP Q9UHN1
D	14	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
D	15	SER	-	CLONING ARTIFACT	UNP Q9UHN1
D	16	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	17	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	18	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	19	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	20	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	21	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	22	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
D	23	SER	-	CLONING ARTIFACT	UNP Q9UHN1
D	24	THR	-	CLONING ARTIFACT	UNP Q9UHN1
D	25	MET	-	CLONING ARTIFACT	UNP Q9UHN1
D	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1

- Molecule 2 is water.

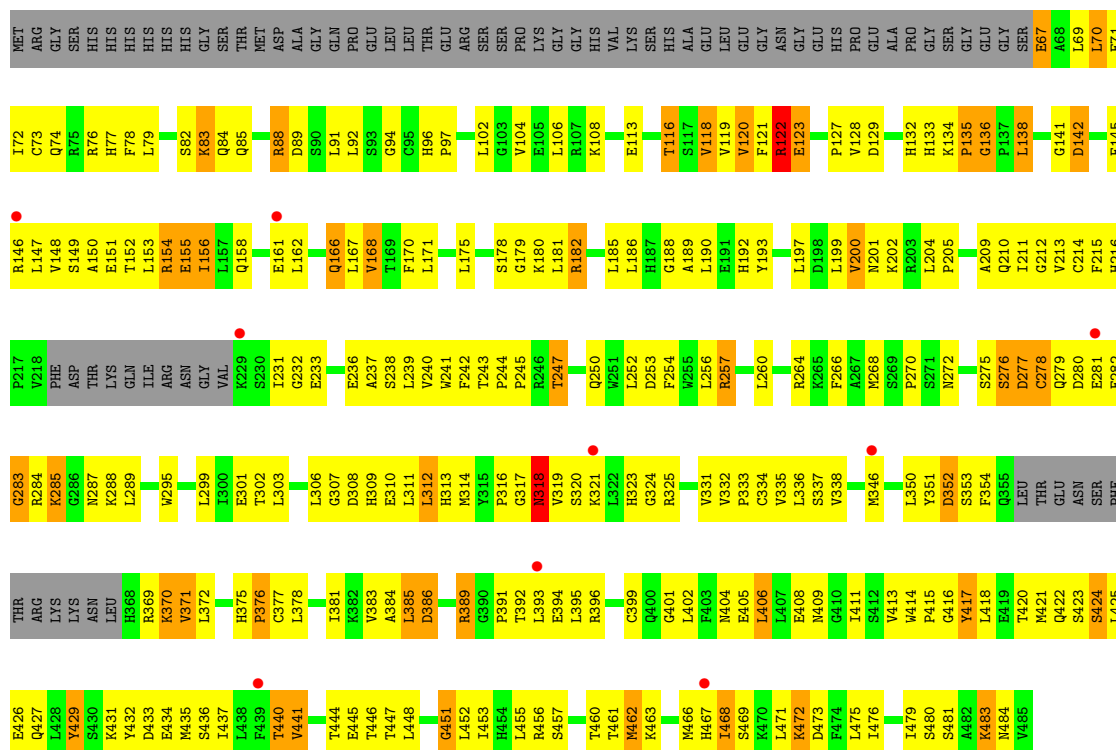
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total 12	O 12	0	0
2	B	5	Total 5	O 5	0	0
2	C	5	Total 5	O 5	0	0
2	D	9	Total 9	O 9	0	0





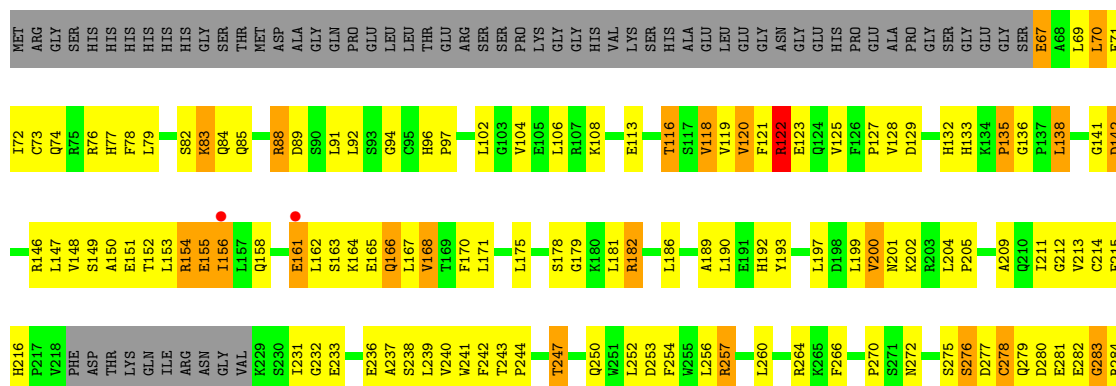
• Molecule 1: DNA polymerase gamma subunit 2

Chain C:



• Molecule 1: DNA polymerase gamma subunit 2

Chain D:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.79Å 101.79Å 170.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.15 48.76 – 3.17	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.15) 95.9 (48.76-3.17)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.285 0.222 , 0.273	Depositor DCC
$R_{free}$ test set	1610 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	91.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 72.5	EDS
Estimated twinning fraction	0.467 for -h,-k,l 0.054 for h,-h-k,-l 0.054 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33607 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.39	0/3278	0.74	3/4432 (0.1%)
1	B	0.39	0/3278	0.74	3/4432 (0.1%)
1	C	0.39	0/3283	0.66	1/4439 (0.0%)
1	D	0.39	0/3283	0.66	1/4439 (0.0%)
All	All	0.39	0/13122	0.70	8/17742 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	NE-CZ-NH1	-13.41	113.59	120.30
1	B	88	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	A	88	ARG	NE-CZ-NH2	13.12	126.86	120.30
1	B	88	ARG	NE-CZ-NH1	13.01	126.80	120.30
1	B	88	ARG	CD-NE-CZ	6.97	133.35	123.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3202	0	3209	276	0
1	B	3202	0	3209	267	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3206	0	3211	289	0
1	D	3206	0	3211	277	0
2	A	12	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	9	0	0	0	0
All	All	12847	0	12840	1063	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

The worst 5 of 1063 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:450:ASN:HD22	1:B:452:LEU:HD23	1.11	1.08
1:A:450:ASN:HD22	1:A:452:LEU:HD23	1.11	1.07
1:A:88:ARG:HD2	1:A:88:ARG:H	1.24	0.98
1:D:306:LEU:HB2	1:D:335:VAL:HG23	1.46	0.98
1:C:306:LEU:HB2	1:C:335:VAL:HG23	1.43	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/474 (82%)	284 (73%)	66 (17%)	41 (10%)	1	6
1	B	391/474 (82%)	284 (73%)	64 (16%)	43 (11%)	1	5
1	C	391/474 (82%)	288 (74%)	72 (18%)	31 (8%)	1	11
1	D	391/474 (82%)	288 (74%)	73 (19%)	30 (8%)	1	12
All	All	1564/1896 (82%)	1144 (73%)	275 (18%)	145 (9%)	1	8

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PHE
1	A	199	LEU
1	A	202	LYS
1	A	282	GLU
1	A	309	HIS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	356/419 (85%)	331 (93%)	25 (7%)	21	65
1	B	356/419 (85%)	330 (93%)	26 (7%)	20	63
1	C	356/419 (85%)	325 (91%)	31 (9%)	15	52
1	D	356/419 (85%)	325 (91%)	31 (9%)	15	52
All	All	1424/1676 (85%)	1311 (92%)	113 (8%)	18	58

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	67	GLU
1	C	241	TRP
1	D	386	ASP
1	C	70	LEU
1	C	122	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	HIS
1	B	313	HIS
1	D	292	ASN
1	B	201	ASN
1	B	258	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	397/474 (83%)	0.07	0 100 100	23, 73, 155, 193	0
1	B	397/474 (83%)	0.07	4 (1%) 79 26	26, 74, 161, 194	0
1	C	397/474 (83%)	0.14	9 (2%) 57 11	28, 80, 163, 202	0
1	D	397/474 (83%)	0.11	4 (1%) 79 26	26, 78, 169, 202	0
All	All	1588/1896 (83%)	0.10	17 (1%) 77 25	23, 77, 162, 202	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	GLU	3.7
1	C	281	GLU	2.7
1	C	229	LYS	2.7
1	B	406	LEU	2.6
1	D	448	LEU	2.4

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.