



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:42 am GMT

PDB ID : 2GV9
Title : Crystal structure of the Herpes Simplex virus type 1 DNA polymerase
Authors : Liu, S.
Deposited on : 2006-05-02
Resolution : 2.68 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

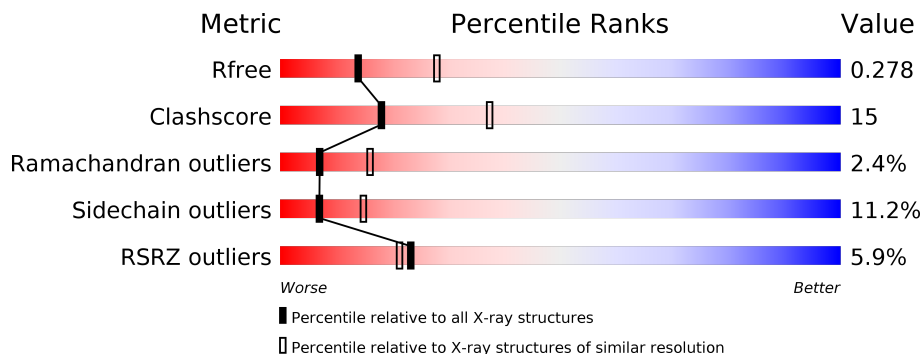
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	100719	3050 (2.70-2.66)
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (2.70-2.66)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1193	<div> <div>7%</div> <div> <div></div> <div>52%</div> <div>25%</div> <div>5%</div> <div>18%</div> </div> </div>
1	B	1193	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>5%</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

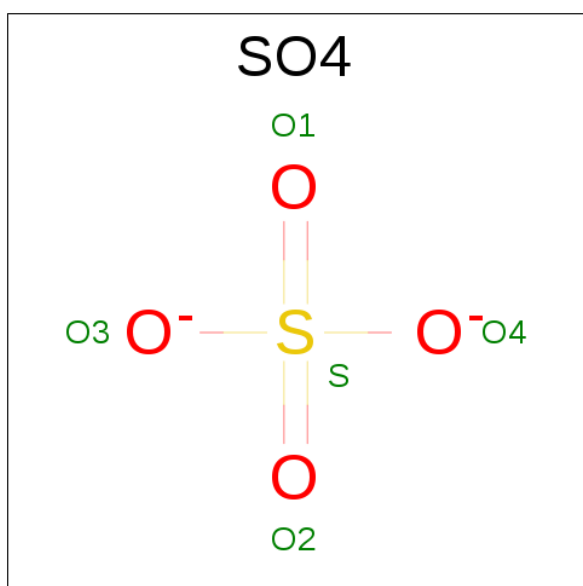
There are 5 unique types of molecules in this entry. The entry contains 16007 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	981	Total	C	N	O	S	0	0	0
			7725	4965	1329	1392	39			
1	B	1035	Total	C	N	O	S	0	0	0
			8180	5247	1422	1471	40			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).

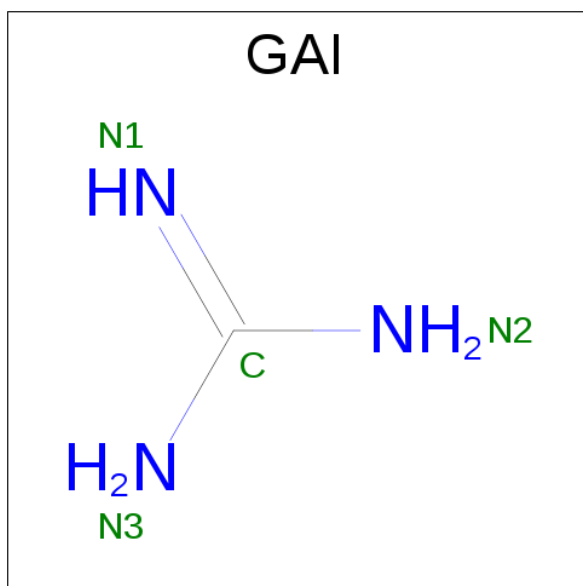


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Hg 1 1	0	0

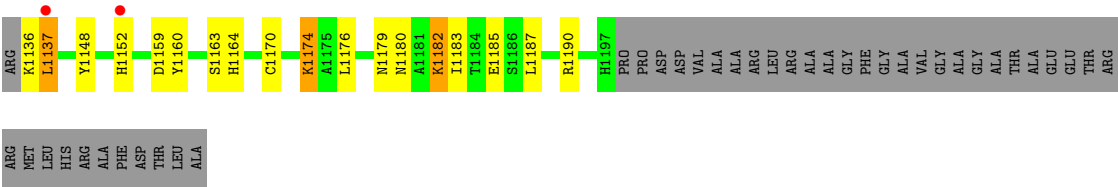
- Molecule 4 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N 4 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	54	Total O 54 54	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.92Å 125.55Å 220.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.68 48.71 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.30-2.68) 98.9 (48.71-2.68)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.281 0.221 , 0.278	Depositor DCC
R_{free} test set	4067 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16007	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, GAI, HG

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	0.81	4/7908 (0.1%)	0.89	16/10727 (0.1%)
1	B	0.90	8/8371 (0.1%)	0.91	13/11352 (0.1%)
All	All	0.86	12/16279 (0.1%)	0.90	29/22079 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	1
All	All	0	8

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	CYS	CB-SG	15.93	2.09	1.82
1	B	262	GLU	CD-OE2	8.40	1.34	1.25
1	A	850	GLU	CG-CD	6.78	1.62	1.51
1	B	1170	CYS	CB-SG	-6.35	1.71	1.82
1	B	578	CYS	CB-SG	-5.58	1.72	1.81

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	920	PRO	C-N-CD	-16.53	84.23	120.60
1	A	920	PRO	C-N-CA	9.82	163.25	122.00
1	A	75	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	126	ARG	NE-CZ-NH2	-7.52	116.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	LEU	CA-CB-CG	7.23	131.93	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	LEU	Peptide
1	A	514	LYS	Peptide
1	A	703	ASP	Peptide
1	A	744	ALA	Peptide
1	A	920	PRO	Peptide

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	7725	0	7706	262	0
1	B	8180	0	8181	220	0
2	B	10	0	0	0	0
3	B	1	0	0	0	0
4	B	4	0	4	0	0
5	A	33	0	0	4	0
5	B	54	0	0	2	0
All	All	16007	0	15891	479	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 15.

The worst 5 of 479 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:A:71:CYS:SG	1:A:71:CYS:CB	2.09	1.41
1:A:501:VAL:HG13	1:A:515:ILE:HG22	1.24	1.16
1:A:898:THR:HG22	1:A:900:ALA:H	1.04	1.09
1:B:501:VAL:HG13	1:B:502:TRP:O	1.51	1.08
1:B:702:LEU:O	1:B:702:LEU:HD23	1.54	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	971/1193 (81%)	865 (89%)	78 (8%)	28 (3%)	5	12
1	B	1027/1193 (86%)	934 (91%)	73 (7%)	20 (2%)	9	21
All	All	1998/2386 (84%)	1799 (90%)	151 (8%)	48 (2%)	7	16

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	SER
1	A	217	GLN
1	A	322	ARG
1	A	376	GLU
1	A	531	ASP

5.3.2 Protein sidechains [i](#)

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	814/971 (84%)	718 (88%)	96 (12%)	6	13
1	B	862/971 (89%)	770 (89%)	92 (11%)	8	16
All	All	1676/1942 (86%)	1488 (89%)	188 (11%)	7	15

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	959	ARG
1	B	196	VAL
1	B	956	ASP
1	A	970	SER
1	A	1192	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1018	HIS
1	B	203	GLN
1	B	1079	GLN
1	A	1152	HIS
1	A	349	ASN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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
2	SO4	B	1236	-	4,4,4	0.30	0	6,6,6	0.36	0
2	SO4	B	1237	-	4,4,4	0.18	0	6,6,6	0.36	0
4	GAI	B	1239	-	3,3,3	1.33	0	3,3,3	0.24	0

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	SO4	B	1236	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1237	-	-	0/0/0/0	0/0/0/0
4	GAI	B	1239	-	-	0/0/0/0	0/0/0/0

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](#)

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, 95th 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 ²)	Q<0.9
1	A	981/1193 (82%)	0.50	82 (8%) 12 9	41, 61, 88, 104	0
1	B	1035/1193 (86%)	0.43	36 (3%) 44 43	39, 60, 85, 99	0
All	All	2016/2386 (84%)	0.47	118 (5%) 23 21	39, 60, 87, 104	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	742	ALA	8.0
1	B	509	PHE	7.2
1	B	217	GLN	6.3
1	B	744	ALA	5.5
1	A	752	TYR	5.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	1236	5/5	0.96	0.12	-2.33	86,89,90,91	0
4	GAI	B	1239	4/4	0.98	0.14	-2.90	41,41,42,42	0
3	HG	B	1238	1/1	0.97	0.03	-	142,142,142,142	0
2	SO4	B	1237	5/5	0.85	0.17	-	111,112,112,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.