



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:59 am BST

PDB ID : 1NB4
Title : HC-J4 RNA polymerase apo-form
Authors : Jaeger, J.; O'Farrell, D.J.; Trowbridge, R.; Rowlands, D.J.
Deposited on : 2002-12-02
Resolution : 2.00 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

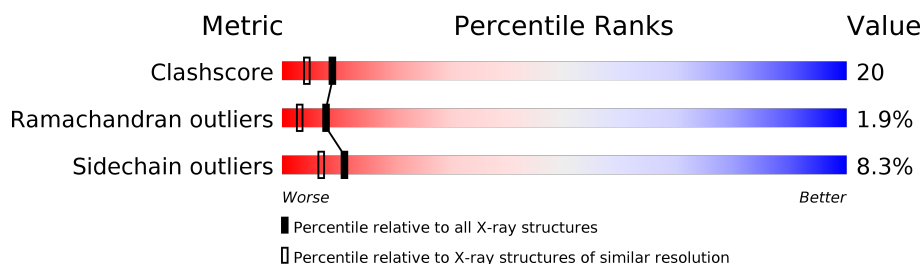
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	570	
1	B	570	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9554 atoms, of which 0 are hydrogens and 0 are deuteriums.

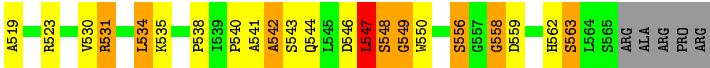
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4388	2763	777	816	32			
1	B	565	Total	C	N	O	S	0	0	0
			4383	2760	776	815	32			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	344	Total	O	0	0
			344	344		
2	B	439	Total	O	0	0
			439	439		



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.69Å 108.71Å 135.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.3 (55.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9554	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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	0.86	2/4484 (0.0%)	0.95	11/6087 (0.2%)
1	B	0.99	3/4479 (0.1%)	0.99	13/6080 (0.2%)
All	All	0.93	5/8963 (0.1%)	0.97	24/12167 (0.2%)

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	1
1	B	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	CYS	CB-SG	-9.77	1.65	1.82
1	B	179	VAL	CB-CG1	-6.55	1.39	1.52
1	B	180	SER	CB-OG	-6.21	1.34	1.42
1	A	52	VAL	CB-CG1	-5.41	1.41	1.52
1	A	261	TYR	CD2-CE2	5.16	1.47	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	B	280	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	A	280	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	280	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	B	259	ARG	NE-CZ-NH2	-9.28	115.66	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	TYR	Sidechain
1	B	383	TYR	Sidechain
1	B	498	ARG	Sidechain

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	4388	0	4383	184	0
1	B	4383	0	4381	173	0
2	A	344	0	0	35	0
2	B	439	0	0	42	0
All	All	9554	0	8764	356	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 20.

The worst 5 of 356 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:B:130:THR:HB	2:B:800:HOH:O	1.31	1.25
1:B:277:ARG:HB3	1:B:277:ARG:HH11	1.14	1.10
1:A:547:LEU:HD12	1:A:565:SER:H	1.06	1.08
1:B:109:ARG:HB2	1:B:109:ARG:NH1	1.72	1.05
1:A:327:ALA:O	1:A:331:GLU:HG3	1.61	1.01

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	564/570 (99%)	532 (94%)	23 (4%)	9 (2%)	9	4
1	B	563/570 (99%)	529 (94%)	22 (4%)	12 (2%)	7	2
All	All	1127/1140 (99%)	1061 (94%)	45 (4%)	21 (2%)	8	3

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	A	540	PRO
1	A	542	ALA
1	A	545	LEU
1	B	103	TYR

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	475/485 (98%)	443 (93%)	32 (7%)	16	11
1	B	475/485 (98%)	428 (90%)	47 (10%)	8	4
All	All	950/970 (98%)	871 (92%)	79 (8%)	11	7

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	LEU
1	B	106	LYS
1	B	498	ARG
1	B	52	VAL
1	B	77	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	ASN
1	B	24	ASN
1	B	483	ASN
1	A	514	GLN
1	B	34	HIS

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](#)

There are no ligands in this entry.

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.