



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:05 AM GMT

PDB ID : 1C2P
Title : HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE
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Deposited on : 1999-07-26
Resolution : 1.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

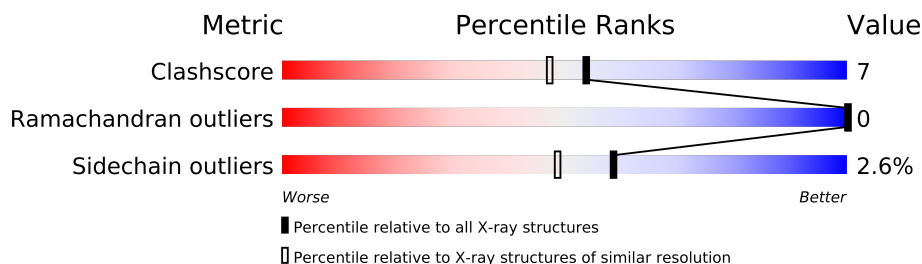
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 1.90 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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9438 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 RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	Se	0	0	0
			4344	2741	769	804	19	11			
1	B	561	Total	C	N	O	S	Se	0	0	0
			4369	2756	775	808	19	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	EXPRESSION TAG	UNP P26663
A	-4	SER	-	EXPRESSION TAG	UNP P26663
A	-3	HIS	-	EXPRESSION TAG	UNP P26663
A	-2	HIS	-	EXPRESSION TAG	UNP P26663
A	-1	HIS	-	EXPRESSION TAG	UNP P26663
A	0	HIS	-	EXPRESSION TAG	UNP P26663
A	1	HIS	-	EXPRESSION TAG	UNP P26663
A	2	HIS	-	EXPRESSION TAG	UNP P26663
A	36	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	71	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	139	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	173	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	187	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	215	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	313	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	329	VAL	THR	CONFLICT	UNP P26663
A	338	ALA	VAL	CONFLICT	UNP P26663
A	343	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	414	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	423	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	426	MSE	MET	MODIFIED RESIDUE	UNP P26663
A	544	GLN	ARG	CONFLICT	UNP P26663
B	-5	ALA	-	EXPRESSION TAG	UNP P26663
B	-4	SER	-	EXPRESSION TAG	UNP P26663
B	-3	HIS	-	EXPRESSION TAG	UNP P26663

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP P26663
B	-1	HIS	-	EXPRESSION TAG	UNP P26663
B	0	HIS	-	EXPRESSION TAG	UNP P26663
B	1	HIS	-	EXPRESSION TAG	UNP P26663
B	2	HIS	-	EXPRESSION TAG	UNP P26663
B	36	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	71	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	139	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	173	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	187	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	215	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	313	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	329	VAL	THR	CONFLICT	UNP P26663
B	338	ALA	VAL	CONFLICT	UNP P26663
B	343	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	414	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	423	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	426	MSE	MET	MODIFIED RESIDUE	UNP P26663
B	544	GLN	ARG	CONFLICT	UNP P26663

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	365	Total O 365 365	0	0
2	B	360	Total O 360 360	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.84Å 105.20Å 127.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.90)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.211 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9438	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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	0.49	0/4429	0.67	1/5993 (0.0%)
1	B	0.52	1/4454 (0.0%)	0.75	7/6026 (0.1%)
All	All	0.50	1/8883 (0.0%)	0.71	8/12019 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	ALA	C-N	9.72	1.56	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	CYS	O-C-N	-17.73	94.33	122.70
1	B	88	ALA	C-N-CA	-7.65	102.57	121.70
1	B	89	CYS	CB-CA-C	-7.16	96.08	110.40
1	B	90	LYS	N-CA-C	-6.53	93.37	111.00
1	B	89	CYS	CA-C-N	6.43	131.35	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	89	CYS	Mainchain

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	4344	0	4357	62	0
1	B	4369	0	4386	59	0
2	A	365	0	0	11	0
2	B	360	0	0	6	0
All	All	9438	0	8743	121	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 7.

The worst 5 of 121 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:CYS:SG	2:A:750:HOH:O	2.06	1.13
1:A:169:VAL:HG12	1:A:173:MSE:HE2	1.35	1.08
1:A:90:LYS:HD2	2:A:884:HOH:O	1.52	1.07
1:B:169:VAL:HG12	1:B:173:MSE:HE2	1.39	1.02
1:B:89:CYS:HB3	1:B:108:VAL:CG1	1.96	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	554/576 (96%)	539 (97%)	15 (3%)	0	100	100
1	B	557/576 (97%)	545 (98%)	12 (2%)	0	100	100
All	All	1111/1152 (96%)	1084 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	475/478 (99%)	464 (98%)	11 (2%)	63	55
1	B	478/478 (100%)	464 (97%)	14 (3%)	55	44
All	All	953/956 (100%)	928 (97%)	25 (3%)	59	49

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	CYS
1	B	47	LEU
1	B	547	LEU
1	B	20	LYS
1	B	57	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	GLN
1	B	544	GLN
1	B	461	GLN
1	A	527	ASN
1	B	527	ASN

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.