



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:05 PM GMT

PDB ID : 1NHV
Title : Hepatitis C virus RNA polymerase in complex with non-nucleoside analogue inhibitor
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Deposited on : 2002-12-19
Resolution : 2.90 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

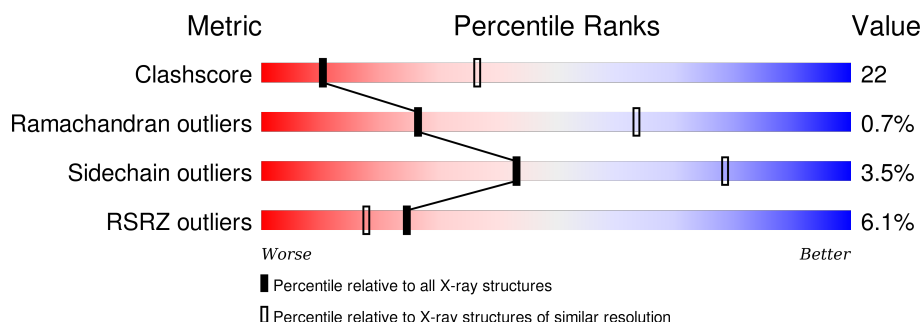
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	578	<div> <div>6%</div> <div>56%</div> <div>39%</div> <div>..</div> </div>
1	B	578	<div> <div>6%</div> <div>59%</div> <div>36%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	154	A	5001	-	-	-	X
2	154	B	6001	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8779 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.

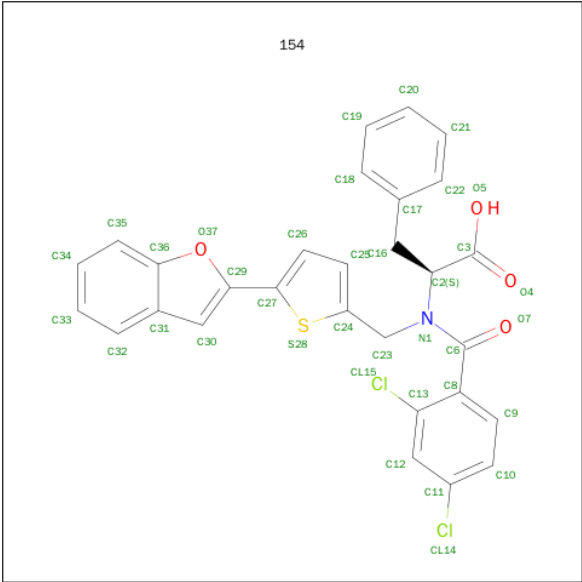
- Molecule 1 is a protein called HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4340	2738	765	806	31			
1	B	561	Total	C	N	O	S	0	0	0
			4365	2753	771	810	31			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	EXPRESSION TAG	UNP P26663
A	-6	SER	-	EXPRESSION TAG	UNP P26663
A	-5	HIS	-	EXPRESSION TAG	UNP P26663
A	-4	HIS	-	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
B	-7	ALA	-	EXPRESSION TAG	UNP P26663
B	-6	SER	-	EXPRESSION TAG	UNP P26663
B	-5	HIS	-	EXPRESSION TAG	UNP P26663
B	-4	HIS	-	EXPRESSION TAG	UNP P26663
B	-3	HIS	-	EXPRESSION TAG	UNP P26663
B	-2	HIS	-	EXPRESSION TAG	UNP P26663
B	-1	HIS	-	EXPRESSION TAG	UNP P26663
B	0	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is (2S)-2-[(5-BENZOFURAN-2-YL-THIOPHEN-2-YLMETHYL)-(2,4-DICHLORO-BENZOYL)-AMINO]-3-PHENYL-PROPIONIC ACID (three-letter code: 154) (formula: C₂₉H₂₁Cl₂NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			37	29	2	1	4	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			37	29	2	1	4	1		

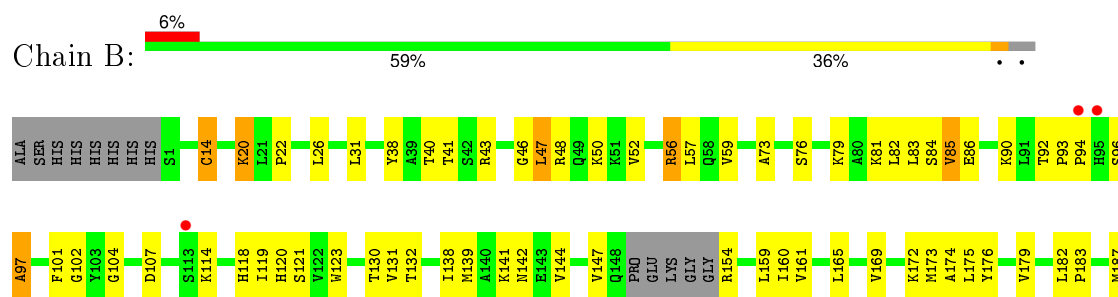
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE



• Molecule 1: HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE



D546	E464	V381	G283	Y191
L547	R465	L384	Q194	Q194
S548	L466	T385	C289	Y195
S549	H467	R386	T294	S196
S550	G468	D387	G295	P197
S551	L469	P388	Y296	G198
S552	S470	T389	L297	Q199
S553	A471	T390	K298	R200
S554	F472	P391	C303	V201
S555	S473	R394	L204	L204
S556	L474	A395	V205	V205
S557	E481	A396	L308	N206
S558	I482	E397	Q309	T207
D559	V485	E398	D310	
I560		T399	C311	N213
S561	V485	A400	T312	P214
H562	C488	R401	K313	H215
H563	L489		L314	G216
S564	R490	N406	V321	F217
S565	K491	S407	V322	S218
S566	L492		I323	Y219
ALA	G493	M414	C324	C223
ARG	V494	Y415	A327	
PRO	P495	A416	G328	S226
ARG	P496	P417	T329	T227
		L419	Q330	N231
	V499	R422	E331	D232
	N500		S335	I233
	R503	M426	L336	R234
	V507	T427	R337	V235
	R508	H428	T340	E236
	A509	I432		I239
	R510	L433	Y346	C242
	L511	L434	S347	C243
	L512		P350	D244
	R517	L439	Q355	A249
	K523	E440	P356	I253
	N527	K441	S365	E258
	V530	A442	C366	Y261
	L534	L443	S367	I262
	K535	D444	S368	N268
	L536	C445	N369	Q272
	T537	Q446	V372	N273
	P538	I447	A373	C274
	I539	Y448	H374	G275
	P540	C451	S377	R280
	A541	I454	G378	
	A542	E455	K379	
	S543	P456	R380	
	Q544	L457		
	L545	D458		
		Q461		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.50Å 107.83Å 126.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 2.90 39.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (39.74-2.90) 94.2 (39.74-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.280 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 25058 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8779	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5035e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 154

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	0.40	0/4434	0.65	0/6017
1	B	0.40	0/4459	0.64	0/6050
All	All	0.40	0/8893	0.64	0/12067

There are no bond length outliers.

There are no bond angle outliers.

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	4340	0	4357	203	0
1	B	4365	0	4386	177	0
2	A	37	0	20	4	0
2	B	37	0	20	0	0
All	All	8779	0	8783	378	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 22.

The worst 5 of 378 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:336:LEU:HD12	1:A:356:PRO:HD3	1.50	0.92
1:B:510:ARG:HG2	1:B:510:ARG:HH11	1.41	0.85
1:A:215:MET:HB2	1:A:326:SER:HB2	1.60	0.83
1:A:192:GLY:HA3	1:A:316:ASN:OD1	1.78	0.82
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.44	0.81

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	554/578 (96%)	508 (92%)	44 (8%)	2 (0%)	39	74
1	B	557/578 (96%)	504 (90%)	47 (8%)	6 (1%)	17	51
All	All	1111/1156 (96%)	1012 (91%)	91 (8%)	8 (1%)	26	63

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	VAL
1	A	90	LYS
1	B	564	LEU
1	A	536	LEU
1	B	97	ALA

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	476/492 (97%)	461 (97%)	15 (3%)	46	81
1	B	479/492 (97%)	461 (96%)	18 (4%)	40	76
All	All	955/984 (97%)	922 (96%)	33 (4%)	43	78

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	510	ARG
1	B	56	ARG
1	B	466	LEU
1	B	14	CYS
1	B	20	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	206	ASN
1	B	231	ASN
1	B	467	HIS
1	B	184	GLN
1	B	527	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

2 ligands are modelled in this entry.

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	154	A	5001	-	32,41,41	2.31	17 (53%)	35,58,58	1.23	5 (14%)
2	154	B	6001	-	32,41,41	2.15	14 (43%)	35,58,58	1.38	6 (17%)

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	154	A	5001	-	-	0/20/28/28	0/4/5/5
2	154	B	6001	-	-	0/20/28/28	0/4/5/5

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6001	154	C19-C18	2.01	1.43	1.38
2	B	6001	154	C12-C11	2.21	1.42	1.38
2	A	5001	154	C12-C13	2.24	1.42	1.38
2	A	5001	154	C12-C11	2.26	1.42	1.38
2	B	6001	154	C12-C13	2.28	1.42	1.38

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6001	154	C12-C13-C8	-3.55	119.22	121.59
2	B	6001	154	O7-C6-C8	-2.56	114.92	120.14
2	A	5001	154	O7-C6-C8	-2.28	115.50	120.14
2	A	5001	154	C12-C13-C8	-2.23	120.10	121.59
2	B	6001	154	C23-N1-C6	2.13	123.22	117.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	154	4	0

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	558/578 (96%)	0.08	34 (6%) 25 18	8, 28, 63, 102	0
1	B	561/578 (97%)	0.20	34 (6%) 25 18	9, 29, 70, 99	0
All	All	1119/1156 (96%)	0.14	68 (6%) 25 18	8, 29, 68, 102	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	GLY	11.1
1	B	563	SER	9.2
1	B	550	TRP	8.8
1	A	550	TRP	8.8
1	A	561	TYR	8.2

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	154	A	5001	37/37	0.81	0.30	2.28	37,44,58,59	0
2	154	B	6001	37/37	0.79	0.35	2.27	40,46,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.