



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 07:05 AM GMT

PDB ID : 1A1V
Title : HEPATITIS C VIRUS NS3 HELICASE DOMAIN COMPLEXED WITH SINGLE STRANDED SDNA
Authors : Kim, J.L.; Morgenstern, K.A.; Griffith, J.P.; Dwyer, M.D.; Thomson, J.A.; Murcko, M.A.; Lin, C.; Caron, P.R.
Deposited on : 1997-12-17
Resolution : 2.20 Å(reported)

This is a full wwPDB validation 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>

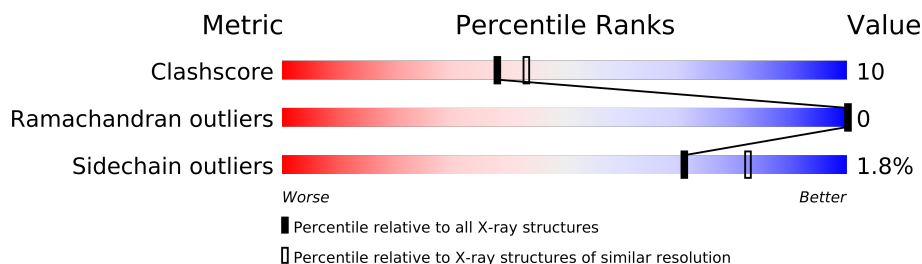
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 Å.

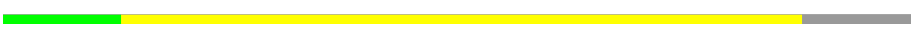

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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	B	8	
2	A	476	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4486 atoms, of which 995 are hydrogens 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 DNA chain called DNA (5'-D(*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	7	Total	C	H	N	O	P	0	0	1
			112	50	5	10	41	6			

- Molecule 2 is a protein called PROTEIN (NS3 PROTEIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	432	Total	C	H	N	O	S	0	0	0
			3892	2047	672	538	612	23			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	ALA	VAL	CONFLICT	UNP P27958
A	248	VAL	ILE	CONFLICT	UNP P27958
A	279	CME	CYS	MODIFIED RESIDUE	UNP P27958
A	418	PHE	TYR	CONFLICT	UNP P27958
A	431	CME	CYS	MODIFIED RESIDUE	UNP P27958
A	449	THR	ILE	CONFLICT	UNP P27958
A	499	CME	CYS	MODIFIED RESIDUE	UNP P27958
A	557	PHE	LEU	CONFLICT	UNP P27958
A	609	VAL	ILE	CONFLICT	UNP P27958
A	615	ILE	VAL	CONFLICT	UNP P27958

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	153	Total	H	O	0	0
			459	306	153		
4	B	6	Total	H	O	0	0
			18	12	6		

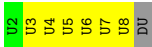
3 Residue-property plots

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.

Note EDS was not executed.


- Molecule 1: DNA (5'-D(*UP*UP*UP*UP*UP*UP*UP*U)-3')

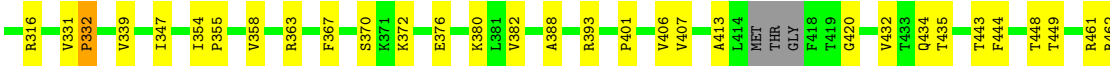
Chain B: 


 U2
U3
U4
U5
U6
U7
U8
DU

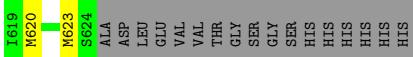
- Molecule 2: PROTEIN (NS3 PROTEIN)

Chain A: 

 MET VAL ASP PHE ILE PRO VAL GLU ASN LEU LEU THR THR MET ARG SER PRO VAL PHE THR ASP ASN SER SER P190 V193 P194 Q195 S196 F197 Q198 A204 K210 V227 L228 N229 P230 V248 R287 I285 T286 Y287 S288 T289 Y270 G271 K272 C279 I287 I300

 R316 V331 P332 V339 I347 I354 P355 V358 R363 F367 S370 K371 K372 E376 K380 L381 V382 A388 R393 P401 V406 V407 A413 L414 MET THR F418 T419 G420 V432 T433 Q434 T435 T443 F444 T448 T449 R461 R462

 G463 R464 T465 G466 K469 R474 F486 V490 W501 T505 P506 A507 R512 L513 R514 A515 T519 G525 L529 G538 H545 F546 S548 Q549 T550 K551 E555 N556 F557 P558 P574 L588 K589 P590 Y600 V605 Q606 N607 T616 R617 Y618

 I619 M620 M623 S624 ALA ASP LEU GLU VAL THR GLY SER GLY HIS HIS HIS HIS HIS HIS

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 2	Depositor
Cell constants a, b, c, α , β , γ	73.10Å 117.50Å 63.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	95.7 (6.00-2.20)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.228 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4486	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CME, SO4

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	B	0.48	0/117	1.08	0/177
2	A	0.39	0/3267	0.65	0/4469
All	All	0.39	0/3384	0.67	0/4646

There are no bond length outliers.

There are no bond angle outliers.

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	B	107	5	52	14	0
2	A	3220	672	2482	61	0
3	A	5	0	0	0	0
4	A	153	306	0	9	0
4	B	6	12	0	0	0
All	All	3491	995	2534	65	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 10.

All (65) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:4:DU:O4	2:A:434:GLN:HG2	1.87	0.75
2:A:194:PRO:O	2:A:316:ARG:HD2	1.90	0.72
1:B:7:DU:H5''	2:A:230:PRO:O	1.89	0.72
2:A:435:THR:HG21	2:A:449:THR:OG1	1.93	0.69
1:B:6:DU:H6	2:A:393:ARG:NH2	2.09	0.68
2:A:501:TRP:CZ2	2:A:551:LYS:HB2	2.30	0.67
2:A:347:ILE:HG23	2:A:380:LYS:HD3	1.78	0.66
2:A:331:VAL:HG13	2:A:332:PRO:HD2	1.79	0.65
2:A:257:ARG:HG3	2:A:257:ARG:HH11	1.62	0.65
1:B:7:DU:H4'	4:A:1003:HOH:H2	1.61	0.64
2:A:512:ARG:HH12	4:A:1053:HOH:H1	1.44	0.63
2:A:355:PRO:O	2:A:358:VAL:HG22	1.98	0.62
1:B:4:DU:H5''	2:A:370:SER:HA	1.84	0.60
2:A:434:GLN:HE22	2:A:448:THR:HG22	1.67	0.60
2:A:229:ASN:O	2:A:269:THR:HA	2.01	0.59
2:A:486:PHE:CZ	2:A:525:CYS:SG	2.95	0.59
2:A:372:LYS:O	2:A:376:GLU:HG3	2.03	0.59
2:A:514:ARG:CZ	2:A:529:LEU:HD12	2.32	0.59
2:A:474:ARG:HH11	4:A:1015:HOH:H2	1.49	0.57
1:B:8:DU:H5'	2:A:271:GLY:HA3	1.88	0.55
2:A:363:ARG:NH1	2:A:420:GLY:O	2.39	0.55
2:A:555:GLU:O	2:A:558:PRO:HD3	2.06	0.55
2:A:204:ALA:HB3	2:A:210:LYS:HD3	1.88	0.55
2:A:574:PRO:HG2	2:A:607:ASN:ND2	2.22	0.55
2:A:505:THR:HG21	4:A:1113:HOH:O	2.07	0.54
2:A:367:PHE:CD2	2:A:461:ARG:HG2	2.43	0.54
2:A:505:THR:HG22	2:A:507:ALA:H	1.72	0.54
2:A:588:LEU:HD21	4:A:1138:HOH:H2	1.75	0.52
2:A:257:ARG:NH1	2:A:257:ARG:HG3	2.23	0.52
2:A:196:SER:O	2:A:198:GLN:HG2	2.10	0.51
2:A:538:GLY:HA3	2:A:618:TYR:CE2	2.45	0.51
2:A:279:CME:HE3	2:A:287:ILE:HD11	1.92	0.51
2:A:505:THR:HG21	4:A:1113:HOH:H2	1.73	0.51
2:A:547:LEU:O	2:A:551:LYS:HG2	2.11	0.51
2:A:474:ARG:HE	4:A:1027:HOH:H1	1.59	0.50
2:A:363:ARG:NH2	2:A:401:PRO:O	2.43	0.50
2:A:605:VAL:HG23	2:A:605:VAL:O	2.12	0.50
1:B:5:DU:OP1	2:A:413:ALA:HB2	2.13	0.49
1:B:5:DU:C2'	2:A:393:ARG:HE	2.25	0.48
2:A:194:PRO:HB2	2:A:196:SER:O	2.13	0.48
2:A:443:THR:HB	2:A:623:MET:HE3	1.94	0.48
2:A:466:GLY:HA2	2:A:469:LYS:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:300:ILE:HD12	2:A:490:VAL:HG11	1.96	0.47
2:A:589:LYS:HB3	2:A:590:PRO:HD3	1.97	0.47
2:A:464:ARG:HH12	4:A:1028:HOH:H2	1.62	0.47
2:A:616:THR:O	2:A:620:MET:HG3	2.16	0.46
2:A:515:ALA:O	2:A:519:THR:HG23	2.15	0.46
2:A:545:HIS:NE2	2:A:549:GLN:OE1	2.49	0.46
1:B:8:DU:H5"	2:A:272:LYS:N	2.31	0.45
2:A:444:PHE:HD2	2:A:623:MET:HE1	1.81	0.45
2:A:193:VAL:CG1	2:A:316:ARG:HG2	2.47	0.44
2:A:248:VAL:HG11	2:A:265:ILE:HD12	2.00	0.44
2:A:388:ALA:HA	2:A:407:VAL:O	2.18	0.42
2:A:462:ARG:HE	4:A:1012:HOH:H2	1.65	0.42
2:A:363:ARG:HA	2:A:406:VAL:O	2.20	0.42
2:A:300:ILE:CD1	2:A:490:VAL:HG11	2.50	0.42
2:A:227:VAL:HB	2:A:267:TYR:CD1	2.56	0.41
1:B:3:DU:H4'	2:A:432:VAL:HG21	2.01	0.41
1:B:5:DU:H2"	2:A:393:ARG:HE	1.84	0.41
1:B:6:DU:H2"	1:B:6:DU:H6	1.74	0.41
2:A:194:PRO:HB3	2:A:198:GLN:HG3	2.02	0.41
1:B:4:DU:H2'	1:B:5:DU:OP2	2.19	0.40
2:A:486:PHE:CE1	2:A:525:CYS:HB3	2.56	0.40
2:A:354:ILE:HA	2:A:355:PRO:HD3	1.85	0.40
1:B:7:DU:H6	1:B:7:DU:H2"	1.68	0.40

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	
2	A	425/476 (89%)	410 (96%)	15 (4%)	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
2	A	340/390 (87%)	334 (98%)	6 (2%)	71 82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	332	PRO
2	A	339	VAL
2	A	382	VAL
2	A	548	SER
2	A	556	ASN
2	A	600	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	198	GLN
2	A	201	HIS
2	A	203	HIS
2	A	434	GLN
2	A	460	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

3 non-standard protein/DNA/RNA residues 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	CME	A	279	2	9,9,10	5.85	2 (22%)	7,9,11	0.75	0
2	CME	A	431	2	9,9,10	5.79	2 (22%)	7,9,11	1.41	1 (14%)
2	CME	A	499	2	9,9,10	5.66	2 (22%)	7,9,11	0.47	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	CME	A	279	2	-	0/6/8/10	0/0/0/0
2	CME	A	431	2	-	0/6/8/10	0/0/0/0
2	CME	A	499	2	-	0/6/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	279	CME	O-C	17.27	1.23	1.11
2	A	431	CME	O-C	17.19	1.23	1.11
2	A	499	CME	O-C	16.84	1.23	1.11
2	A	279	CME	CA-C	2.92	1.53	1.48
2	A	499	CME	CA-C	2.24	1.52	1.48
2	A	431	CME	CA-C	2.19	1.52	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	431	CME	C-CA-N	-3.60	110.24	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
3	SO4	A	1001	-	4,4,4	0.67	0	6,6,6	0.54	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
3	SO4	A	1001	-	-	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.

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.