

wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 07:10 pm BST

PDB ID : 3M5O

Title : Crystal structure of HCV NS3/4A protease in complex with N-terminal prod-

uct 5A5B

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Deposited on : 2010-03-12

Resolution : 1.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

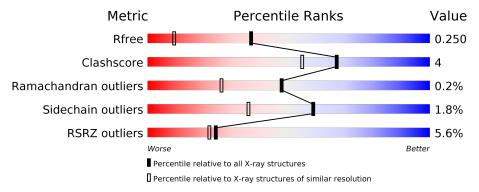
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.60 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	203	94%	
1	В	203	90%	7% •
2	С	8	100%	
2	D	8	25%	



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3526 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 NS3/4A.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	108	Total	С	N	О	S	0	4	0
1	A	198	1478	915	271	284	8	0	4	U
1	D	198	Total	С	N	О	S	0	4	0
1	Б	190	1470	911	271	280	8	0	4	U

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	980	GLY	_	EXPRESSION TAG	UNP A8DG50
A	981	SER	_	EXPRESSION TAG	UNP A8DG50
A	982	HIS	_	EXPRESSION TAG	UNP A8DG50
A	983	MET	_	EXPRESSION TAG	UNP A8DG50
A	984	ALA	-	EXPRESSION TAG	UNP A8DG50
A	985	SER	-	EXPRESSION TAG	UNP A8DG50
A	986	MET	-	ENGINEERED MUTATION	UNP A8DG50
A	987	LYS	-	ENGINEERED MUTATION	UNP A8DG50
A	988	LYS	-	ENGINEERED MUTATION	UNP A8DG50
A	989	LYS	-	ENGINEERED MUTATION	UNP A8DG50
A	991	SER	CYS	SEE REMARK 999	UNP A8DG50
A	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
A	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
A	1001	SER	ALA	ENGINEERED MUTATION	UNP A8DG50
A	1002	GLY	PRO	ENGINEERED MUTATION	UNP A8DG50
A	1003	ASP	ILE	ENGINEERED MUTATION	UNP A8DG50
A	1013	GLU	LEU	ENGINEERED MUTATION	UNP A8DG50
A	1014	GLU	LEU	ENGINEERED MUTATION	UNP A8DG50
A	1017	GLN	ILE	ENGINEERED MUTATION	UNP A8DG50
A	1018	GLU	ILE	ENGINEERED MUTATION	UNP A8DG50
A	1021	GLN	LEU	ENGINEERED MUTATION	UNP A8DG50
A	1040	THR	ALA	ENGINEERED MUTATION	UNP A8DG50
A	1047	SER	CYS	ENGINEERED MUTATION	UNP A8DG50
A	1052	LEU	CYS	ENGINEERED MUTATION	UNP A8DG50
A	1072	THR	ILE	ENGINEERED MUTATION	UNP A8DG50

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1086	GLN	PRO	ENGINEERED MUTATION	UNP A8DG50
A	1139	ALA	SER	ENGINEERED MUTATION	UNP A8DG50
A	1159	SER	CYS	ENGINEERED MUTATION	UNP A8DG50
В	980	GLY	_	EXPRESSION TAG	UNP A8DG50
В	981	SER	_	EXPRESSION TAG	UNP A8DG50
В	982	HIS	-	EXPRESSION TAG	UNP A8DG50
В	983	MET	-	EXPRESSION TAG	UNP A8DG50
В	984	ALA	_	EXPRESSION TAG	UNP A8DG50
В	985	SER	-	EXPRESSION TAG	UNP A8DG50
В	986	MET	_	ENGINEERED MUTATION	UNP A8DG50
В	987	LYS	-	ENGINEERED MUTATION	UNP A8DG50
В	988	LYS	-	ENGINEERED MUTATION	UNP A8DG50
В	989	LYS	_	ENGINEERED MUTATION	UNP A8DG50
В	991	SER	CYS	SEE REMARK 999	UNP A8DG50
В	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
В	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
В	1001	SER	ALA	ENGINEERED MUTATION	UNP A8DG50
В	1002	GLY	PRO	ENGINEERED MUTATION	UNP A8DG50
В	1003	ASP	ILE	ENGINEERED MUTATION	UNP A8DG50
В	1013	GLU	LEU	ENGINEERED MUTATION	UNP A8DG50
В	1014	GLU	LEU	ENGINEERED MUTATION	UNP A8DG50
В	1017	GLN	ILE	ENGINEERED MUTATION	UNP A8DG50
В	1018	GLU	ILE	ENGINEERED MUTATION	UNP A8DG50
В	1021	GLN	LEU	ENGINEERED MUTATION	UNP A8DG50
В	1040	THR	ALA	ENGINEERED MUTATION	UNP A8DG50
В	1047	SER	CYS	ENGINEERED MUTATION	UNP A8DG50
В	1052	LEU	CYS	ENGINEERED MUTATION	UNP A8DG50
В	1072	THR	ILE	ENGINEERED MUTATION	UNP A8DG50
В	1086	GLN	PRO	ENGINEERED MUTATION	UNP A8DG50
В	1139	ALA	SER	ENGINEERED MUTATION	UNP A8DG50
В	1159	SER	CYS	ENGINEERED MUTATION	UNP A8DG50

 \bullet Molecule 2 is a protein called TEDVVCC peptide.

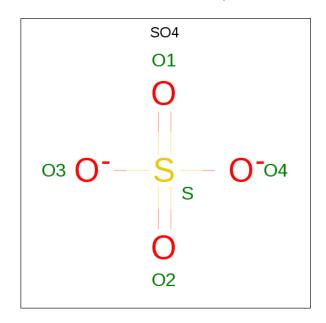
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	С	0	Total	С	N	О	S	0	0	0
		0	54	31	7	14	2	U	U	U
9	D	0	Total	С	N	О	S	0	0	0
		8	54	31	7	14	2	U	U	0

There are 2 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	${f Comment}$	Reference
С	0	ACE	-	ACETYLATION	UNP B3TKQ3
D	0	ACE	=	ACETYLATION	UNP B3TKQ3

 \bullet Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



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

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
4	В	1	Total Zn 1 1	0	0
4	A	1	Total Zn 1 1	0	0

 \bullet Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	257	Total O 257 257	0	0
5	В	186	Total O 186 186	0	0
5	С	10	Total O 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	10	Total O 10 10	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: NS3/4A

Chain A:

94%

• Molecule 1: NS3/4A

Chain B:

90%

7%

7%

• Molecule 1: NS3/4A

• Molecule 2: TEDVVCC peptide

Chain C: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: TEDVVCC peptide

Chain D: 100%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	47.27Å 58.88Å 67.06Å	Depositor
a, b, c, α , β , γ	90.00° 99.22° 90.00°	Depositor
Resolution (Å)	50.00 - 1.60	Depositor
Resolution (A)	22.00 - 1.60	EDS
% Data completeness	94.4 (50.00-1.60)	Depositor
(in resolution range)	94.4 (22.00-1.60)	EDS
R_{merge}	0.05	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	8.39 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
P. P.	0.180 , 0.226	Depositor
R, R_{free}	0.220 , 0.250	DCC
R_{free} test set	2294 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41, 46.5	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3526	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.34% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: ZN, SO4, ACE

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.47	0/1515	0.65	1/2056~(0.0%)	
1	В	0.41	0/1507	0.65	0/2046	
2	С	0.47	0/51	0.56	0/68	
2	D	0.31	0/51	0.61	0/68	
All	All	0.44	0/3124	0.65	1/4238 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	1130	ARG	NE-CZ-NH1	5.53	123.07	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1478	0	1487	11	0
1	В	1470	0	1479	13	0
2	С	54	0	48	0	0
2	D	54	0	48	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0

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Continued	trom	nromanne	naae
-	110116	picolous	puyc

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	1	0	0	0	0
5	A	257	0	0	0	0
5	В	186	0	0	1	0
5	С	10	0	0	0	0
5	D	10	0	0	0	0
All	All	3526	0	3062	24	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 4.

The worst 5 of 24 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:1114:ILE:HD11	1:A:1134:TYR:HE2	1.46	0.80
1:B:1042:THR:HG21	1:B:1109:ARG:HH22	1.45	0.79
1:B:1117:ARG:CG	1:B:1127:LEU:HD21	2.13	0.79
1:B:1042:THR:HG22	1:B:1109:ARG:HH12	1.49	0.76
1:B:1117:ARG:HG2	1:B:1127:LEU:HD21	1.74	0.69

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	Perce	ntiles
1	A	200/203~(98%)	198 (99%)	2 (1%)	0	100	100
1	В	200/203 (98%)	195 (98%)	4 (2%)	1 (0%)	29	11
2	С	6/8 (75%)	6 (100%)	0	0	100	100
2	D	6/8 (75%)	6 (100%)	0	0	100	100
All	All	412/422 (98%)	405 (98%)	6 (2%)	1 (0%)	47	26



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	1001	SER

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	Perce	ntiles
1	A	161/164 (98%)	157 (98%)	4 (2%)	47	22
1	В	159/164 (97%)	156 (98%)	3 (2%)	57	34
2	С	7/7 (100%)	7 (100%)	0	100	100
2	D	7/7 (100%)	7 (100%)	0	100	100
All	All	334/342 (98%)	327 (98%)	7 (2%)	59	29

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1130	ARG
1	В	1165	LYS
1	В	1066	SER
1	A	1109[A]	ARG
1	В	1114	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	В	ond leng	$_{ m gths}$	Е	ond ang	gles
WIOI	Mol Type Chain R	res	S LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	SO4	A	1	_	4,4,4	0.17	0	6,6,6	0.17	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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	198/203 (97%)	0.46	8 (4%) 38 35	11, 18, 44, 81	0
1	В	198/203 (97%)	0.66	13 (6%) 18 17	13, 22, 46, 79	0
2	С	7/8 (87%)	0.18	0 100 100	18, 19, 26, 26	0
2	D	7/8 (87%)	1.14	2 (28%) 0 0	23, 24, 40, 41	0
All	All	410/422 (97%)	0.56	23 (5%) 24 22	11, 20, 44, 81	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	985	SER	4.9
1	В	1001	SER	4.7
1	В	984	ALA	3.8
1	В	1002	GLY	3.4
1	В	1016	CYS	3.1

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. The B-factors column lists the minimum, median, 95^{th} 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	${f B-factors}({f \AA}^2)$	Q<0.9
3	SO4	A	1	5/5	0.92	0.18	32,34,35,35	0
4	ZN	В	2	1/1	0.97	0.07	23,23,23,23	0
4	ZN	A	1183	1/1	0.99	0.05	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.

