



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 08:37 am BST

PDB ID : 6MWN
Title : Crystal structure of hepatitis A virus IRES domain V in complex with Fab HAVx
Authors : Koirala, D.; Shao, Y.; Piccirilli, J.A.
Deposited on : 2018-10-29
Resolution : 2.84 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
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

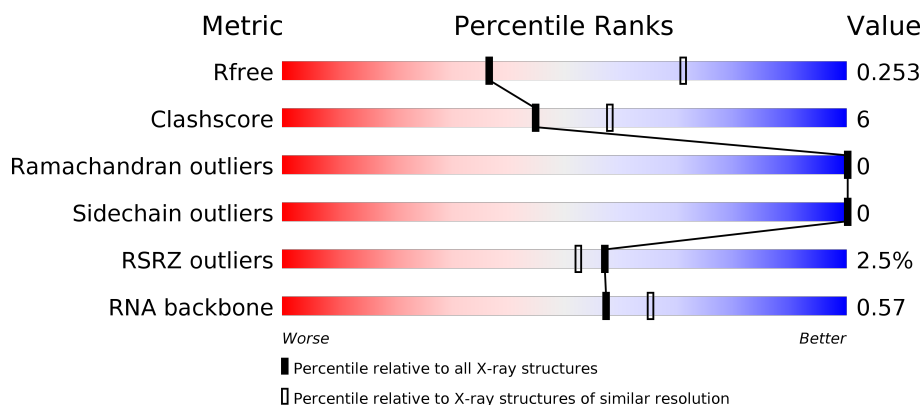
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)
RNA backbone	3102	1077 (3.10-2.58)

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 $\leq 5\%$. 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	92	
1	B	92	
2	C	258	
2	H	258	

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Mol	Chain	Length	Quality of chain
3	D	238	<div><div>%</div><div><div></div><div>79%</div><div>11%</div><div>11%</div></div></div>
3	L	238	<div><div></div><div><div>77%</div><div>13%</div><div>11%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10810 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 RNA chain called HAV dV RNA (92-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	P	0	0	0
			1967	873	336	664	94			
1	B	92	Total	C	N	O	P	0	0	0
			1967	873	336	664	94			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	593	GTP	-	insertion	GB 329582
B	593	GTP	-	insertion	GB 329582

- Molecule 2 is a protein called Fab HAVx Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	225	Total	C	N	O	S	0	0	0
			1686	1067	281	332	6			
2	H	225	Total	C	N	O	S	0	0	0
			1686	1067	281	332	6			

- Molecule 3 is a protein called Fab HAVx Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	213	Total	C	N	O	S	0	0	0
			1662	1043	282	332	5			
3	L	213	Total	C	N	O	S	0	0	0
			1662	1043	282	332	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		

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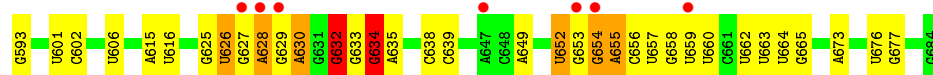
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	41	Total 41	O 41	0	0
4	C	16	Total 16	O 16	0	0
4	D	19	Total 19	O 19	0	0
4	H	30	Total 30	O 30	0	0
4	L	40	Total 40	O 40	0	0

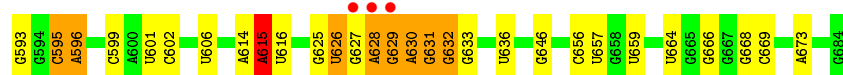
3 Residue-property plots [i](#)

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.

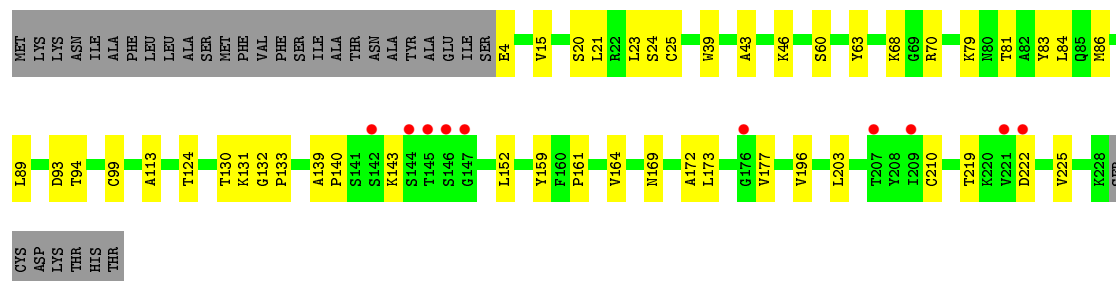
- Molecule 1: HAV dV RNA (92-MER)



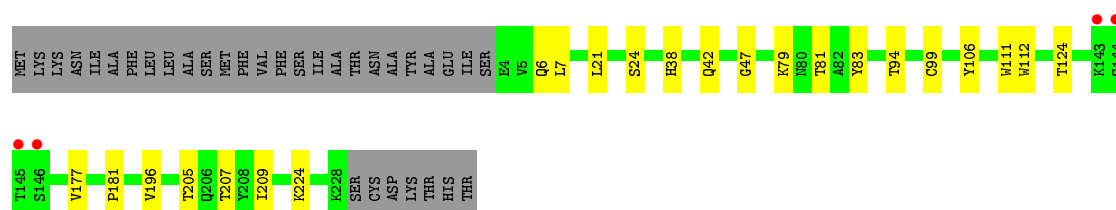
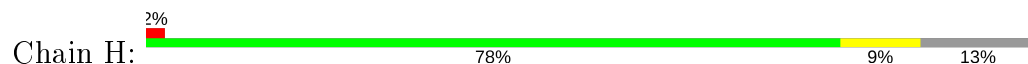
- Molecule 1: HAV dV RNA (92-MER)



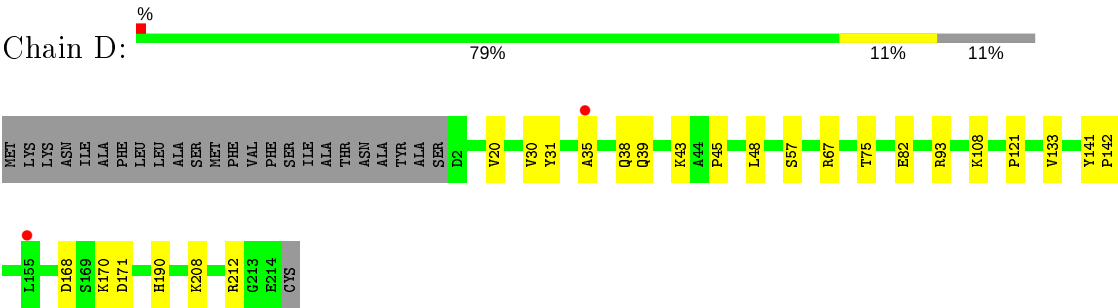
- Molecule 2: Fab HAVx Heavy Chain



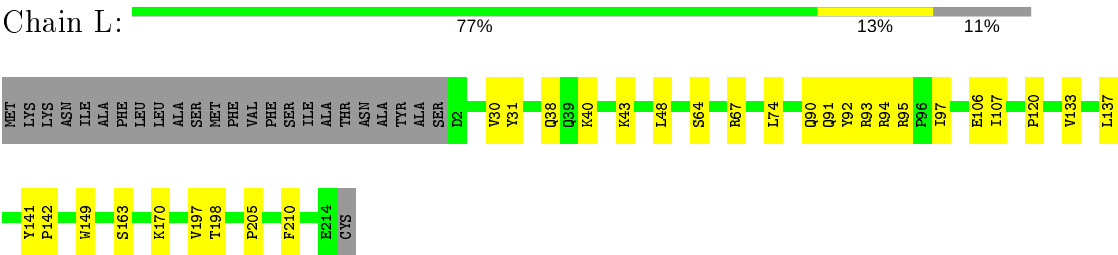
- Molecule 2: Fab HAVx Heavy Chain



● Molecule 3: Fab HAVx Light Chain



● Molecule 3: Fab HAVx Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	74.15Å 100.58Å 236.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.84 29.61 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.61-2.84) 99.6 (29.61-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.85Å)	Xtriage
Refinement program	PHENIX (1.14)	Depositor
R, R_{free}	0.186 , 0.252 0.185 , 0.253	Depositor DCC
R_{free} test set	1718 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å ²)	100.0	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 30.78 % 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 1.2344e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GTP

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	0.58	5/2160 (0.2%)	0.96	0/3364
1	B	0.83	7/2160 (0.3%)	1.17	0/3364
2	C	0.41	0/1731	0.60	0/2361
2	H	0.45	0/1731	0.65	0/2361
3	D	0.45	0/1699	0.66	0/2305
3	L	0.53	0/1699	0.71	0/2305
All	All	0.57	12/11180 (0.1%)	0.86	0/16060

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	633	G	O3'-P	-7.95	1.51	1.61
1	B	664	U	O3'-P	-7.54	1.52	1.61
1	B	668	G	O3'-P	-7.11	1.52	1.61
1	B	615	A	O3'-P	-6.56	1.53	1.61
1	B	669	C	O3'-P	-6.31	1.53	1.61

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	1967	0	983	21	0
1	B	1967	0	983	14	0
2	C	1686	0	1642	34	0
2	H	1686	0	1642	15	0
3	D	1662	0	1620	18	0
3	L	1662	0	1620	21	0
4	A	34	0	0	0	0
4	B	41	0	0	1	0
4	C	16	0	0	1	0
4	D	19	0	0	0	0
4	H	30	0	0	1	0
4	L	40	0	0	0	0
All	All	10810	0	8490	113	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 6.

The worst 5 of 113 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)
2:C:133:PRO:HB3	2:C:159:TYR:HB3	1.59	0.84
1:B:628:A:N3	1:B:629:G:N2	2.37	0.72
3:L:198:THR:HG22	3:L:205:PRO:HB3	1.71	0.71
2:C:15:VAL:HG21	2:C:21:LEU:HG	1.72	0.70
2:C:70:ARG:NH2	2:C:93:ASP:OD2	2.24	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	Percentiles
2	C	223/258 (86%)	212 (95%)	11 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	223/258 (86%)	214 (96%)	9 (4%)	0	100	100
3	D	211/238 (89%)	203 (96%)	8 (4%)	0	100	100
3	L	211/238 (89%)	204 (97%)	7 (3%)	0	100	100
All	All	868/992 (88%)	833 (96%)	35 (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	C	188/216 (87%)	188 (100%)	0	100	100
2	H	188/216 (87%)	188 (100%)	0	100	100
3	D	189/209 (90%)	189 (100%)	0	100	100
3	L	189/209 (90%)	189 (100%)	0	100	100
All	All	754/850 (89%)	754 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	90/92 (97%)	16 (17%)	2 (2%)
1	B	90/92 (97%)	14 (15%)	2 (2%)
All	All	180/184 (97%)	30 (16%)	4 (2%)

5 of 30 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	606	U
1	A	615	A
1	A	616	U
1	A	626	U
1	A	627	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	652	U
1	A	659	U
1	B	595	C
1	B	626	U

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 [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	91/92 (98%)	0.29	7 (7%) 13 8	79, 133, 231, 286	0
1	B	91/92 (98%)	-0.27	3 (3%) 46 39	59, 78, 142, 271	0
2	C	225/258 (87%)	0.26	10 (4%) 34 26	56, 105, 189, 248	0
2	H	225/258 (87%)	-0.18	4 (1%) 68 63	50, 78, 116, 215	0
3	D	213/238 (89%)	0.10	2 (0%) 84 83	53, 102, 161, 181	0
3	L	213/238 (89%)	-0.25	0 100 100	46, 66, 94, 122	0
All	All	1058/1176 (89%)	-0.01	26 (2%) 57 52	46, 84, 177, 286	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	146	SER	13.4
2	C	147	GLY	11.4
2	C	145	THR	10.3
2	C	144	SER	7.5
1	A	629	G	7.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.