



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 10:38 PM EST

PDB ID : 4L3B  
Title : X-ray structure of the HRV2 A particle uncoating intermediate  
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Deposited on : 2013-06-05  
Resolution : 6.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

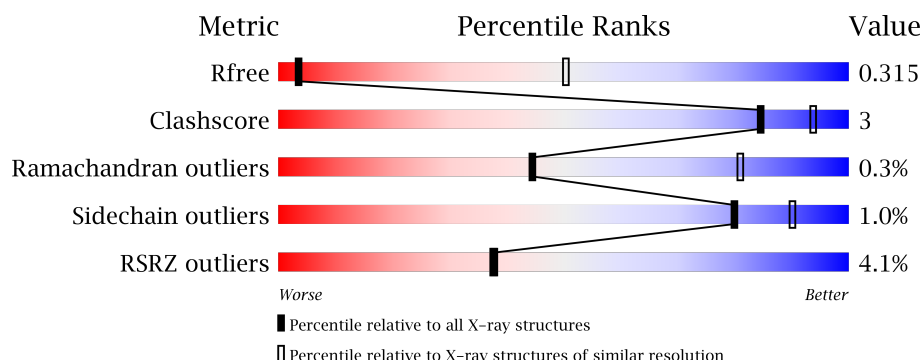
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 6.50 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))
$R_{free}$	100719	1098 (9.00-3.70)
Clashscore	112137	1031 (9.00-3.80)
Ramachandran outliers	110173	1000 (9.00-3.76)
Sidechain outliers	110143	1096 (9.00-3.70)
RSRZ outliers	101464	1000 (9.00-3.72)

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  $\geq 3$ , 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	289	
2	B	261	
3	C	237	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5514 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 Protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1772	1126	310	325	11			

- Molecule 2 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1911	1218	328	357	8			

- Molecule 3 is a protein called Protein VP3.

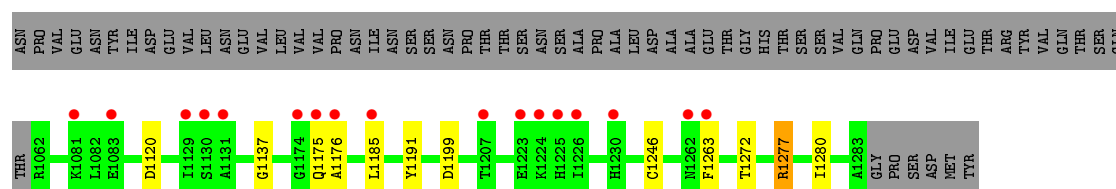
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1831	1169	304	346	12			

### 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.

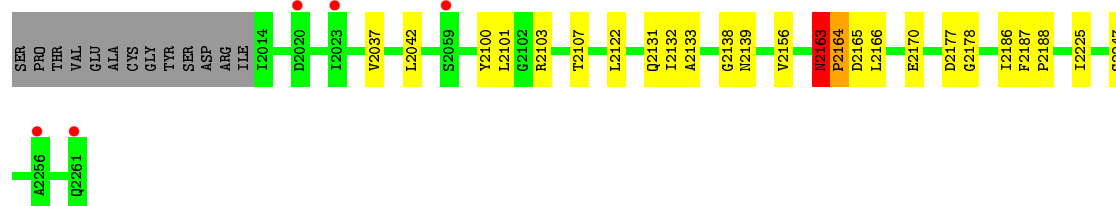
#### • Molecule 1: Protein VP1

Chain A: 



#### • Molecule 2: Protein VP2

Chain B: 



#### • Molecule 3: Protein VP3

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	311.93Å 357.83Å 386.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.39 – 6.50 121.39 – 4.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (121.39-6.50) 12.3 (121.39-4.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 4.47Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.309 , 0.320 0.315 , 0.315	Depositor DCC
$R_{free}$ test set	775 reflections (5.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.8	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 558.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	5514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	343.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.28	0/1820	0.49	2/2474 (0.1%)
2	B	0.31	1/1966 (0.1%)	0.50	1/2690 (0.0%)
3	C	0.29	0/1881	0.44	0/2575
All	All	0.29	1/5667 (0.0%)	0.48	3/7739 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2164	PRO	N-CD	5.16	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1199	ASP	N-CA-C	6.77	129.28	111.00
1	A	1246	CYS	N-CA-C	6.72	129.16	111.00
2	B	2163	ASN	C-N-CD	5.83	140.65	128.40

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	1772	0	1694	5	0
2	B	1911	0	1824	17	0
3	C	1831	0	1804	11	0
All	All	5514	0	5322	29	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 3.

All (29) 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:B:2163:ASN:HB3	2:B:2164:PRO:CD	1.97	0.91
2:B:2100:TYR:O	2:B:2101:LEU:HD23	1.84	0.77
2:B:2037:VAL:HG21	3:C:3037:PRO:HB3	1.65	0.76
2:B:2163:ASN:HB3	2:B:2164:PRO:HD2	1.79	0.64
2:B:2165:ASP:CG	2:B:2166:LEU:H	2.05	0.59
2:B:2122:LEU:HD21	2:B:2225:ILE:HG23	1.87	0.57
3:C:3014:LEU:HD23	3:C:3017:ASP:HB3	1.90	0.54
2:B:2165:ASP:O	2:B:2166:LEU:C	2.47	0.53
2:B:2186:ILE:HA	3:C:3049:VAL:HG11	1.90	0.53
2:B:2107:THR:HB	2:B:2247:SER:HB3	1.95	0.47
3:C:3055:ILE:HG21	3:C:3070:VAL:HG22	1.95	0.47
1:A:1175:GLN:HG2	1:A:1176:ALA:H	1.80	0.46
2:B:2131:GLN:H	2:B:2177:ASP:HA	1.81	0.46
1:A:1277:ARG:HG3	1:A:1280:ILE:HG22	1.98	0.45
2:B:2163:ASN:HB3	2:B:2164:PRO:HD3	1.90	0.45
3:C:3153:VAL:HG21	3:C:3165:MET:HG3	1.99	0.44
1:A:1185:LEU:HB2	1:A:1191:TYR:HE2	1.84	0.43
2:B:2042:LEU:HD22	2:B:2103:ARG:HD3	2.01	0.43
2:B:2156:VAL:HG13	2:B:2170:GLU:HB3	2.00	0.43
3:C:3146:ASP:HA	3:C:3149:LEU:HD12	2.00	0.43
2:B:2187:PHE:O	2:B:2188:PRO:C	2.56	0.42
3:C:3087:THR:HG21	3:C:3133:TYR:HE1	1.83	0.42
1:A:1263:PHE:H	2:B:2133:ALA:HB2	1.84	0.42
3:C:3117:PHE:HD1	3:C:3210:CYS:HA	1.85	0.42
3:C:3140:GLU:HA	3:C:3141:PRO:HD3	1.88	0.42
3:C:3054:PRO:HA	3:C:3068:TYR:HA	2.01	0.41
1:A:1263:PHE:HZ	2:B:2178:GLY:HA2	1.84	0.41
2:B:2138:GLY:O	2:B:2139:ASN:C	2.58	0.40
3:C:3130:LEU:HD13	3:C:3147:ALA:HB1	2.02	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	
1	A	220/289 (76%)	200 (91%)	19 (9%)	1 (0%)	32	74
2	B	246/261 (94%)	204 (83%)	41 (17%)	1 (0%)	38	77
3	C	235/237 (99%)	214 (91%)	21 (9%)	0	100	100
All	All	701/787 (89%)	618 (88%)	81 (12%)	2 (0%)	44	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2163	ASN
1	A	1137	GLY

### 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	187/257 (73%)	184 (98%)	3 (2%)	68	85
2	B	205/226 (91%)	204 (100%)	1 (0%)	91	95
3	C	209/210 (100%)	207 (99%)	2 (1%)	80	90
All	All	601/693 (87%)	595 (99%)	6 (1%)	80	90

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

Mol	Chain	Res	Type
1	A	1120	ASP

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Mol	Chain	Res	Type
1	A	1272	THR
1	A	1277	ARG
2	B	2132	ILE
3	C	3004	VAL
3	C	3050	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2131	GLN
2	B	2218	HIS
3	C	3073	GLN
3	C	3231	GLN

### 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 ⓘ

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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	222/289 (76%)	0.55	17 (7%)	14 20	228, 343, 500, 500	0
2	B	248/261 (95%)	0.15	5 (2%)	65 63	58, 336, 500, 500	7 (2%)
3	C	237/237 (100%)	0.05	7 (2%)	51 49	226, 320, 452, 500	0
All	All	707/787 (89%)	0.24	29 (4%)	38 38	58, 332, 500, 500	7 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	3236	ALA	6.8
1	A	1174	GLY	6.6
3	C	3237	GLN	5.5
1	A	1207	THR	3.6
3	C	3175	TYR	3.6
1	A	1223	GLU	3.5
3	C	3235	ILE	3.2
2	B	2059	SER	3.1
1	A	1131	ALA	3.1
1	A	1263	PHE	2.9
2	B	2256	ALA	2.9
1	A	1225	HIS	2.8
1	A	1176	ALA	2.7
1	A	1083	GLU	2.7
3	C	3176	ARG	2.7
1	A	1224	LYS	2.6
3	C	3222	MET	2.6
1	A	1130	SER	2.6
1	A	1129	ILE	2.5
1	A	1230	HIS	2.5
1	A	1226	ILE	2.5
2	B	2023	ILE	2.4
1	A	1081	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	2261	GLN	2.3
1	A	1262	ASN	2.2
1	A	1175	GLN	2.1
1	A	1185	LEU	2.1
3	C	3027	TRP	2.0
2	B	2020	ASP	2.0

## 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.