



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:52 AM UTC

PDB ID : 4L3B / pdb_00004l3b
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

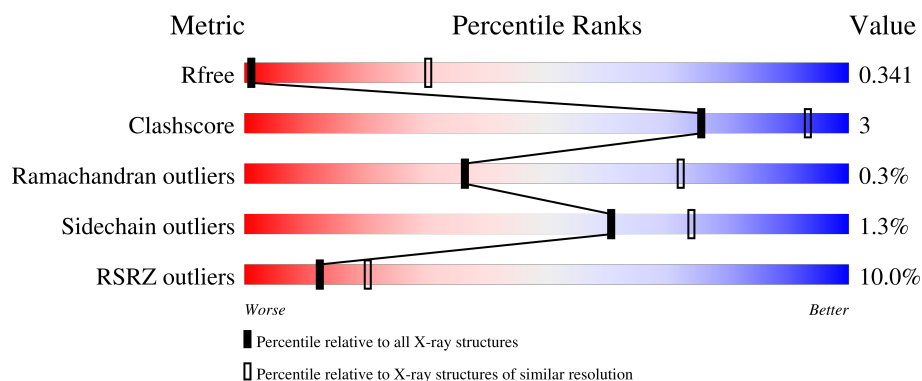
1 Overall quality at a glance

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}	180053	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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 of 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	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
			Total	C	N	O	S			
1	A	222	1772	1126	310	325	11	0	0	0

- Molecule 2 is a protein called Protein VP2.

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

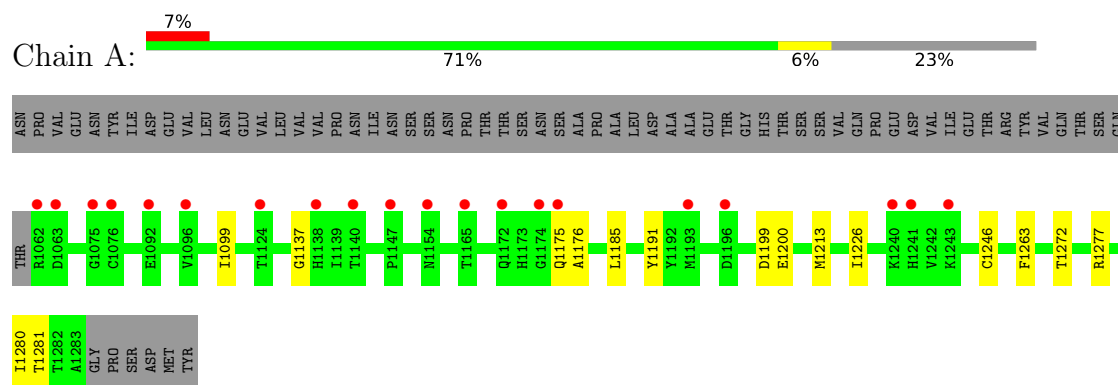
- Molecule 3 is a protein called Protein VP3.

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

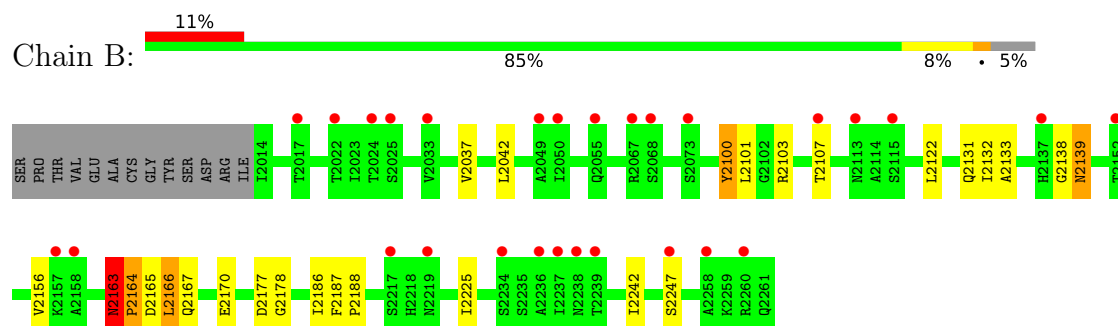
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

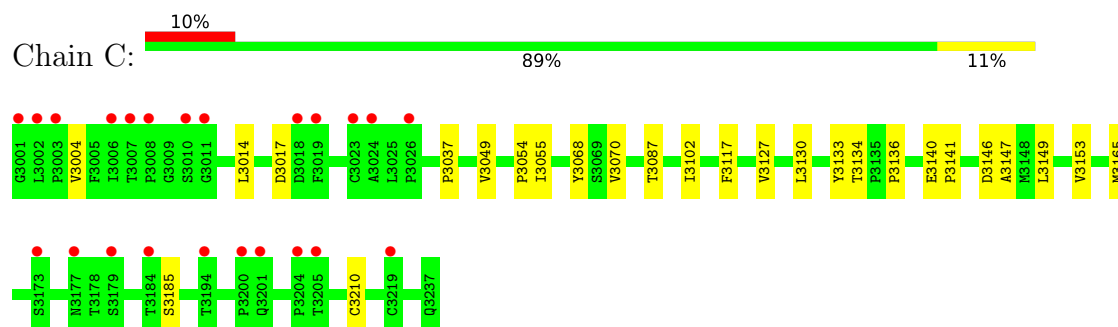
• Molecule 1: Protein VP1



• Molecule 2: Protein VP2



• Molecule 3: Protein VP3



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	311.93Å 357.83Å 386.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.39 – 6.50 121.39 – 6.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (121.39-6.50) 30.2 (121.39-6.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.47Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.309 , 0.320 0.332 , 0.341	Depositor DCC
R_{free} test set	813 reflections (0.64%)	wwPDB-VP
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.11	EDS
Total number of atoms	5514	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	0.39	0/1820	0.77	4/2474 (0.2%)
2	B	0.41	1/1966 (0.1%)	0.78	7/2690 (0.3%)
3	C	0.42	0/1881	0.71	2/2575 (0.1%)
All	All	0.41	1/5667 (0.0%)	0.75	13/7739 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2164	PRO	N-CD	5.23	1.55	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2100	TYR	N-CA-C	12.10	124.02	111.07
1	A	1246	CYS	N-CA-C	8.75	129.16	109.81
1	A	1199	ASP	N-CA-C	8.68	129.28	110.80
1	A	1200	GLU	N-CA-C	-7.20	103.94	114.39
2	B	2166	LEU	N-CA-C	-6.83	100.53	110.64
2	B	2166	LEU	CB-CA-C	6.66	117.99	109.80
2	B	2139	ASN	CB-CA-C	6.50	118.74	109.71
2	B	2100	TYR	CB-CA-C	-5.68	101.97	110.88
2	B	2163	ASN	CA-C-N	-5.28	113.24	119.84
2	B	2163	ASN	C-N-CA	-5.28	113.24	119.84
1	A	1281	THR	N-CA-C	-5.22	107.93	114.56
3	C	3134	THR	CA-C-N	5.03	123.33	119.66
3	C	3134	THR	C-N-CA	5.03	123.33	119.66

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	6	0
2	B	1911	0	1824	18	0
3	C	1831	0	1804	12	0
All	All	5514	0	5322	32	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 (32) 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	0.64
2:B:2165:ASP:O	2:B:2166:LEU:C	2.47	0.58
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:2186:ILE:HA	3:C:3049:VAL:HG11	1.90	0.53
1:A:1099:ILE:HB	1:A:1213:MET:HE3	1.91	0.52
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
2:B:2187:PHE:O	2:B:2188:PRO:C	2.56	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:2138:GLY:O	2:B:2139:ASN:C	2.58	0.45
2:B:2165:ASP:CG	2:B:2166:LEU:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:3136:PRO:HB3	3:C:3185:SER:C	2.46	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 [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	220/289 (76%)	200 (91%)	19 (9%)	1 (0%)	24	63
2	B	246/261 (94%)	204 (83%)	41 (17%)	1 (0%)	30	67
3	C	235/237 (99%)	214 (91%)	21 (9%)	0	100	100
All	All	701/787 (89%)	618 (88%)	81 (12%)	2 (0%)	36	72

All (2) Ramachandran outliers are listed below:

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

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	187/257 (73%)	185 (99%)	2 (1%)	65	76
2	B	205/226 (91%)	202 (98%)	3 (2%)	57	72
3	C	209/210 (100%)	206 (99%)	3 (1%)	59	72
All	All	601/693 (87%)	593 (99%)	8 (1%)	61	74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1226	ILE
1	A	1272	THR
2	B	2132	ILE
2	B	2167	GLN
2	B	2242	ILE
3	C	3004	VAL
3	C	3102	ILE
3	C	3127	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1078	HIS
1	A	1227	HIS
2	B	2061	ASN
2	B	2131	GLN
2	B	2141	ASN
2	B	2175	ASN
2	B	2218	HIS
2	B	2238	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	222/289 (76%)	0.52	20 (9%)	15 22	228, 343, 500, 500	0
2	B	248/261 (95%)	0.60	28 (11%)	10 18	58, 336, 498, 500	7 (2%)
3	C	237/237 (100%)	0.39	23 (9%)	13 21	226, 320, 452, 500	0
All	All	707/787 (89%)	0.51	71 (10%)	12 20	58, 332, 499, 500	7 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1241	HIS	6.7
2	B	2236	ALA	6.2
2	B	2024	THR	5.7
1	A	1174	GLY	5.7
3	C	3026	PRO	5.7
2	B	2107	THR	4.4
3	C	3023	CYS	4.3
3	C	3205	THR	4.3
2	B	2025	SER	4.1
1	A	1096	VAL	4.1
2	B	2067	ARG	4.0
1	A	1076	CYS	4.0
1	A	1062	ARG	3.9
2	B	2247	SER	3.9
3	C	3010	SER	3.9
1	A	1172	GLN	3.9
3	C	3006	ILE	3.8
2	B	2115	SER	3.8
3	C	3184	THR	3.6
1	A	1175	GLN	3.6
3	C	3002	LEU	3.6
1	A	1240	LYS	3.6
1	A	1154	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	3008	PRO	3.5
1	A	1165	THR	3.4
3	C	3007	THR	3.3
3	C	3003	PRO	3.3
2	B	2158	ALA	3.2
2	B	2073	SER	3.2
2	B	2239	THR	3.2
3	C	3024	ALA	3.0
1	A	1138	HIS	3.0
3	C	3201	GLN	3.0
2	B	2237	ILE	3.0
2	B	2219	ASN	3.0
2	B	2137	HIS	2.9
2	B	2260	ARG	2.9
1	A	1063	ASP	2.9
2	B	2055	GLN	2.8
2	B	2113	ASN	2.8
1	A	1147	PRO	2.8
2	B	2152	THR	2.8
2	B	2157	LYS	2.7
3	C	3179	SER	2.7
3	C	3173	SER	2.7
3	C	3018	ASP	2.6
1	A	1075	GLY	2.6
1	A	1243	LYS	2.5
1	A	1140	THR	2.5
2	B	2017	THR	2.4
2	B	2234	SER	2.4
3	C	3177	ASN	2.4
3	C	3019	PHE	2.4
2	B	2217	SER	2.4
3	C	3200	PRO	2.3
3	C	3001	GLY	2.3
1	A	1193	MET	2.3
3	C	3219	CYS	2.2
2	B	2033	VAL	2.2
2	B	2258	ALA	2.2
3	C	3011	GLY	2.2
1	A	1196	ASP	2.2
1	A	1092	GLU	2.1
1	A	1124	THR	2.1
2	B	2050	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	2049	ALA	2.1
2	B	2238	ASN	2.1
3	C	3204	PRO	2.1
2	B	2022	THR	2.1
3	C	3194	THR	2.1
2	B	2068	SER	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 oligosaccharides 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.