



## Full wwPDB EM Validation Report ⓘ

Jan 13, 2025 – 06:36 PM JST

PDB ID : 9JJI  
EMDB ID : EMD-61528  
Title : Local refinement of RHDV GI.2 T=1 VLP  
Authors : Ruan, Z.; Shao, Q.; Song, Y.; Hu, B.; Fan, Z.; Wei, H.; Liu, Y.; Wang, F.; Fang, Q.  
Deposited on : 2024-09-13  
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM 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

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

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

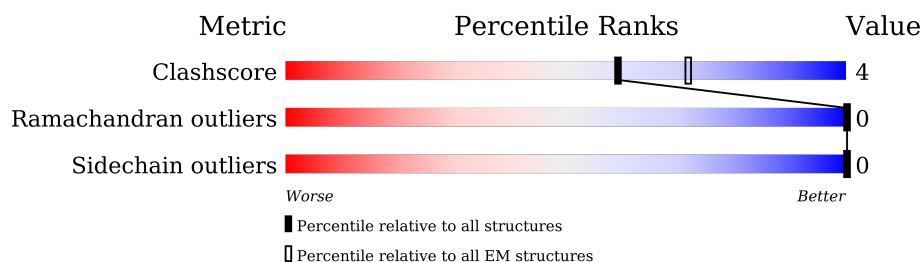
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*





The reported resolution of this entry is 3.40 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	542	
1	B	542	
1	C	542	
1	D	542	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10021 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	168	Total	C	N	O	S	0	0
			1298	837	218	238	5		
1	B	492	Total	C	N	O	S	0	0
			3673	2344	615	702	12		
1	C	168	Total	C	N	O	S	0	0
			1298	837	218	238	5		
1	D	504	Total	C	N	O	S	0	0
			3752	2389	628	723	12		

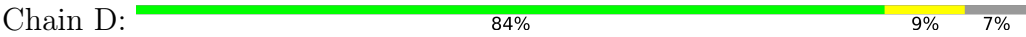
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	MET	VAL	conflict	UNP A0A3S8Q1D6
A	347	ILE	THR	conflict	UNP A0A3S8Q1D6
B	62	MET	VAL	conflict	UNP A0A3S8Q1D6
B	347	ILE	THR	conflict	UNP A0A3S8Q1D6
C	62	MET	VAL	conflict	UNP A0A3S8Q1D6
C	347	ILE	THR	conflict	UNP A0A3S8Q1D6
D	62	MET	VAL	conflict	UNP A0A3S8Q1D6
D	347	ILE	THR	conflict	UNP A0A3S8Q1D6



SER	TYR	VAL	LEU	ASN	LYS	ALA	PRO	ASP	HIS	THR	R161	SER
ASN	THR	ASN	PHE	THR	ASN	ILE	MET	ASN	ASN	VAL	Y162	THR
ALA	PRO	ILE	ALA	PRO	VAL	ALA	PHE	LEU	ASN	THR	L173	THR
SER	ILE	MET	THR	PHE	SER	LYS	VAL	GLY	GLY	GLU	V194	GLU
PHE	PHE	ASN	GLY	ASN	ILE	ILE	PHE	SER	THR	THR	L198	ASN
MET	ALA	THR	GLU	SER	VAL	GLY	SER	GLY	TYR	TYR	I199	ALA
GLU	SER	VAL	LEU	VAL	GLY	GLY	ILE	THR	GLY	GLY	N200	SER
THR	ASN	THR	GLY	VAL	ASN	ASN	THR	THR	THR	THR	G203	THR
VAL	THR	THR	VAL	ARG	THR	THR	THR	THR	SER	SER	S218	ALA
ASP	GLY	GLY	ASP	GLY	GLY	ILE	ALA	ALA	ARG	ARG	E219	THR
GLY	TYR	ILE	TYR	ASN	ASN	GLN	GLY	ALA	PHE	PHE	T233	ALA
PHE	PHE	ASN	PHE	ASN	THR	THR	THR	TRP	ALA	ALA	VAL	GLY
ALA	ALA	GLU	ALA	GLY	ALA	ALA	GLY	GLY	ASP	ASP	ASP	ILE
GLY	GLY	ALA	GLY	ALA	GLY	GLY	PHE	PHE	HIS	HIS	ILE	PRO
THR	THR	GLY	THR	GLY	GLY	LEU	GLY	GLY	ASP	ASP	SER	PRO
GLY	GLY	SER	GLY	SER	PHE	PHE	GLY	GLY	ARG	ARG	PRO	GLN
THR	THR	ASN	SER	ASN	MET	MET	TRP	TRP	ASN	ASN	ALA	GLN
ALA	GLY	GLY	ALA	GLY	ALA	ALA	ASN	ALA	ALA	ALA	LEU	ASP
THR	THR	THR	THR	THR	THR	SER	SER	SER	SER	SER	LEU	GLN
LEU	LEU	GLN	LEU	GLN	GLY	GLY	SER	SER	PHE	PHE	THR	THR
ILE	ILE	TYR	ILE	TYR	VAL	VAL	ASN	ASN	PRO	PRO	THR	THR
ASP	GLY	GLY	ASP	GLY	ILE	ILE	GLY	GLY	GLY	GLY	PRO	THR
LEU	LEU	ALA	LEU	ALA	SER	SER	ALA	ALA	SER	VAL	W68	VAL
SER	SER	GLY	SER	GLY	THR	THR	PRO	PRO	SER	SER	LEU	THR
ASP	ASP	SER	ASP	SER	THR	ASN	TYR	TYR	THR	THR	V82	THR
LEU	LEU	GLN	LEU	GLN	ASN	ASN	VAL	VAL	SER	GLY	GLY	THR
VAL	VAL	PRO	VAL	PRO	PRO	SER	THR	THR	ASN	VAL	A85	THR
ASP	ASP	LEU	ASP	LEU	SER	SER	THR	THR	VAL	GLY	GLY	THR
ILE	ILE	PRO	ILE	PRO	ALA	ALA	MET	LEU	VAL	THR	S96	THR
ARG	VAL	PRO	ARG	VAL	THR	THR	GLN	GLU	GLU	ASP	P97	THR
PRO	PRO	THR	PRO	THR	THR	THR	ALA	LEU	ASN	ASN	Q98	THR
VAL	ILE	ILE	VAL	ILE	THR	TYR	TYR	THR	TRP	ARG	N99	THR
GLY	GLY	THR	GLY	THR	THR	THR	GLU	TRP	TYR	TRP	THR	THR
PRO	PRO	LEU	PRO	LEU	PRO	PRO	LEU	GLY	TYR	ASN	T103	THR
ARG	SER	SER	ARG	SER	SER	GLN	GLY	SER	ALA	GLY	A104	THR
PRO	LEU	PRO	PRO	LEU	THR	PRO	PHE	ALA	ALA	GLU	V105	THR
SER	ASN	ASN	SER	ASN	ASN	ARG	ALA	THR	SER	ILE	L106	THR
THR	THR	THR	THR	THR	VAL	ILE	THR	THR	VAL	VAL	G130	THR
VAL	VAL	VAL	VAL	SER	ASN	VAL	PRO	ASP	GLN	LEU	L133	THR
VAL	VAL	ALA	VAL	ASN	ALA	ALA	SER	ASN	ASN	PRO	I138	THR
ASN	LEU	PRO	ASN	LEU	PRO	GLY	ASN	PRO	ILE	PRO	VAL	THR
LEU	ASN	MET	LEU	THR	PRO	THR	GLN	GLN	GLY	GLY	I144	THR
GLY	GLY	GLY	GLY	GLN	GLY	ALA	THR	THR	ILE	GLY	L148	THR
THR	THR	PHE	THR	ALA	ALA	ALA	THR	THR	ALA	THR	F149	THR
THR	THR	PHE	THR	ALA	ALA	ALA	THR	THR	PRO	THR	V150	THR
ASN	ASN	VAL	ASN	VAL	PRO	PRO	THR	THR	ASP	THR	CYS	THR
PHE	PHE	TRP	PHE	TRP	ILE	ILE	SER	SER	PHE	GLY	D159	THR
GLY	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	THR	ARG	A160	THR

● Molecule 1: Capsid protein



THR	SER	VAL	THR	GLU	ASN	ALA	THR	SER	THR	ILE	ALA	THR	ALA	GLY	ILE	GLY	GLY	PRO	PRO	GLN	GLN	MET	ASP	GLN	GLN	E66	T67	W68	F72	D76	V77	E214	M225	I226	R227	S231	T244	T245	P246	T249	N255	I261	V262	R276	H277	W278		
S289	P290	R291	G300	S309	L315	D325	F336	V355	W361	P368	L378	K402	G410	I411	N412	Q413	A416	M421	S427	M430	S431	S432	F463	A464	S465	T495	L500	L507	Q511	D546	L547	L550	I553	R559														
L569	GLY	GLY	THR	THR	ASN	GLY	PHE	SER	TYR	VAL																																						

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70159	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	26.09	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.31	0/1338	0.53	0/1835
1	B	0.31	0/3781	0.50	0/5192
1	C	0.33	0/1338	0.51	0/1835
1	D	0.30	0/3862	0.49	0/5304
All	All	0.31	0/10319	0.50	0/14166

There are no bond length outliers.

There are no bond angle outliers.

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	1298	0	1266	9	0
1	B	3673	0	3540	38	0
1	C	1298	0	1266	15	0
1	D	3752	0	3619	30	0
All	All	10021	0	9691	87	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.

All (87) 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)
1:D:309:SER:HB2	1:D:410:GLY:H	1.54	0.72
1:A:110:TYR:O	1:A:227:ARG:NH1	2.25	0.69
1:B:374:GLN:HE21	1:B:405:TYR:HB2	1.58	0.69
1:A:159:ASP:OD1	1:A:160:ALA:N	2.26	0.68
1:B:374:GLN:NE2	1:B:405:TYR:HB2	2.10	0.67
1:B:426:ILE:HD12	1:B:437:THR:HG21	1.77	0.66
1:D:66:GLU:OE1	1:D:68:TRP:NE1	2.26	0.66
1:D:361:TRP:HA	1:D:368:PRO:HA	1.78	0.63
1:C:105:VAL:HG13	1:C:106:LEU:HD12	1.83	0.61
1:B:315:LEU:HD12	1:B:402:LYS:HD2	1.82	0.61
1:D:546:ASP:OD1	1:D:547:LEU:N	2.34	0.60
1:A:66:GLU:OE1	1:A:68:TRP:NE1	2.28	0.60
1:B:246:PRO:HA	1:B:249:THR:HG22	1.85	0.59
1:B:304:PHE:HD2	1:B:312:VAL:HG21	1.68	0.58
1:B:465:SER:O	1:B:486:GLY:N	2.32	0.56
1:C:82:VAL:HG12	1:C:198:LEU:HD22	1.87	0.56
1:D:227:ARG:NH1	1:D:231:SER:OG	2.36	0.56
1:B:110:TYR:O	1:B:227:ARG:NH1	2.37	0.56
1:D:278:TRP:HD1	1:D:495:THR:HG23	1.71	0.56
1:C:96:SER:O	1:C:99:ASN:ND2	2.39	0.55
1:B:392:THR:HA	1:B:444:VAL:HG22	1.89	0.55
1:B:280:LEU:HD12	1:B:530:VAL:HA	1.89	0.55
1:D:255:ASN:ND2	1:D:276:ARG:O	2.39	0.54
1:B:418:LEU:HD12	1:B:419:PHE:H	1.73	0.54
1:C:200:ASN:OD1	1:C:203:GLY:N	2.41	0.54
1:A:97:PRO:O	1:A:103:THR:OG1	2.22	0.53
1:D:355:VAL:HG21	1:D:427:SER:HB3	1.89	0.53
1:C:173:LEU:HD22	1:D:225:MET:HE2	1.91	0.52
1:B:267:VAL:HG12	1:B:270:GLY:H	1.76	0.50
1:B:468:ARG:NH1	1:B:473:ILE:O	2.45	0.49
1:C:66:GLU:OE1	1:C:68:TRP:NE1	2.37	0.49
1:B:431:SER:HB2	1:B:481:ASN:HD21	1.78	0.49
1:D:261:ILE:HD12	1:D:463:PHE:HB3	1.95	0.49
1:C:138:ILE:HG21	1:C:144:ILE:HD11	1.94	0.48
1:B:105:VAL:O	1:B:108:GLN:HG3	2.14	0.48
1:D:550:LEU:HD21	1:D:553:ILE:HD11	1.94	0.48
1:D:244:THR:HG22	1:D:246:PRO:HD2	1.95	0.48
1:D:278:TRP:HE1	1:D:290:PRO:HG3	1.78	0.47
1:B:172:ASP:OD1	1:B:174:ARG:NH1	2.39	0.47
1:A:90:LEU:HD11	1:A:194:VAL:HG23	1.96	0.47
1:D:300:GLY:O	1:D:416:ALA:N	2.43	0.47
1:B:224:VAL:HG23	1:B:225:MET:H	1.79	0.47

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:ASN:ND2	1:D:432:SER:OG	2.48	0.47
1:D:336:PHE:CE2	1:D:378:LEU:HD23	2.50	0.46
1:D:507:LEU:HD22	1:D:511:GLN:HB2	1.97	0.46
1:B:255:ASN:ND2	1:B:276:ARG:O	2.47	0.46
1:D:278:TRP:CD1	1:D:495:THR:HG23	2.50	0.46
1:D:262:VAL:HG22	1:D:465:SER:HA	1.96	0.46
1:B:457:LYS:NZ	1:B:539:GLY:HA3	2.31	0.46
1:B:463:PHE:CE1	1:B:491:PRO:HD3	2.50	0.46
1:B:256:ARG:HB3	1:B:257:TRP:CD1	2.50	0.45
1:A:76:ASP:OD1	1:A:77:VAL:N	2.50	0.45
1:B:251:VAL:HG21	1:D:500:LEU:HD21	1.99	0.45
1:B:159:ASP:OD1	1:B:160:ALA:N	2.50	0.44
1:C:148:LEU:HD23	1:C:150:VAL:HG22	1.99	0.44
1:A:120:ARG:HG3	1:A:167:THR:HG22	2.00	0.44
1:B:100:ASN:ND2	1:B:217:PRO:HD3	2.32	0.44
1:B:274:CYS:HB3	1:B:449:THR:HG21	2.00	0.44
1:D:315:LEU:HG	1:D:402:LYS:HB2	2.00	0.44
1:B:523:PHE:HB3	1:C:85:ALA:HB2	2.00	0.43
1:D:559:ARG:HD3	1:D:559:ARG:HA	1.76	0.43
1:B:341:PHE:HB3	1:B:381:ALA:HB2	1.99	0.43
1:B:431:SER:CB	1:B:481:ASN:HD21	2.31	0.43
1:D:76:ASP:OD1	1:D:77:VAL:N	2.50	0.43
1:B:321:GLY:HA2	1:B:331:ILE:HA	2.00	0.43
1:C:130:GLY:O	1:C:198:LEU:HA	2.19	0.43
1:D:411:ILE:HG22	1:D:413:GLN:HG2	2.00	0.42
1:C:159:ASP:OD1	1:C:161:ARG:HG2	2.19	0.42
1:C:159:ASP:HB3	1:C:162:SER:HB3	2.01	0.42
1:B:298:ASP:HA	1:B:417:GLY:HA2	2.00	0.42
1:B:224:VAL:HG23	1:B:225:MET:N	2.34	0.42
1:B:170:MET:HE1	1:B:190:LEU:HB2	2.00	0.42
1:A:224:VAL:HG23	1:A:225:MET:N	2.35	0.41
1:D:245:THR:HA	1:D:553:ILE:HD13	2.02	0.41
1:D:245:THR:O	1:D:249:THR:OG1	2.26	0.41
1:B:361:TRP:CE2	1:B:417:GLY:HA3	2.55	0.41
1:C:218:SER:OG	1:C:219:GLU:N	2.53	0.41
1:B:423:SER:HB2	1:D:421:MET:HE1	2.01	0.41
1:B:148:LEU:HD12	1:B:148:LEU:HA	1.91	0.41
1:C:133:LEU:HD23	1:C:194:VAL:HA	2.02	0.41
1:A:152:GLN:HB2	1:B:228:ALA:HB2	2.02	0.41
1:B:326:ASN:OD1	1:B:328:ILE:HG22	2.21	0.40
1:C:97:PRO:O	1:C:103:THR:OG1	2.27	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ASP:N	1:D:325:ASP:OD1	2.54	0.40
1:B:418:LEU:HD12	1:B:419:PHE:N	2.36	0.40
1:D:72:PHE:HB3	1:D:214:GLU:HB3	2.03	0.40
1:D:289:SER:O	1:D:291:ARG:N	2.54	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 PDB entries followed by that with respect to all EM entries.

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	166/542 (31%)	163 (98%)	3 (2%)	0	100	100
1	B	486/542 (90%)	474 (98%)	12 (2%)	0	100	100
1	C	166/542 (31%)	163 (98%)	3 (2%)	0	100	100
1	D	502/542 (93%)	486 (97%)	16 (3%)	0	100	100
All	All	1320/2168 (61%)	1286 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	142/435 (33%)	142 (100%)	0	100	100
1	B	395/435 (91%)	395 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	142/435 (33%)	142 (100%)	0	100	100
1	D	406/435 (93%)	406 (100%)	0	100	100
All	All	1085/1740 (62%)	1085 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	481	ASN

### 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 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.