Full wwPDB EM Validation Report

Jan 13, 2025 – 06:37 PM JST

PDB ID	:	9JJG
EMDB ID	:	EMD-61526
Title	:	Cryo-EM structure of RHDV GI.2 virion
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	:	2.46 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*
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:

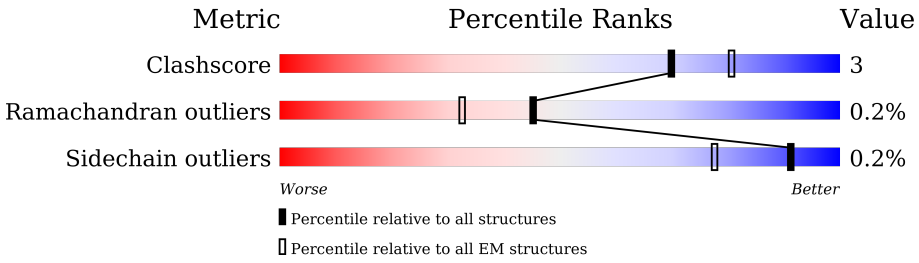
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 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 >=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%

Mol	Chain	Length	Quality of chain
1	A	579	82% 7% 11%
1	B	579	84% 8% 7%
1	C	579	87% 7% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11818 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	515	Total	C	N	O	S	0	0
			3833	2438	643	739	13		
1	B	537	Total	C	N	O	S	0	0
			3978	2524	666	774	14		
1	C	541	Total	C	N	O	S	0	0
			4007	2542	670	781	14		

There are 6 discrepancies between the modelled and reference sequences:

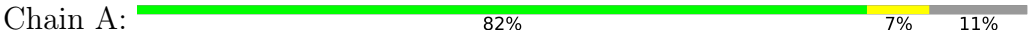
Chain	Residue	Modelled	Actual	Comment	Reference
A	62	MET	VAL	conflict	UNP A0A3S8Q1D6
A	347	ILE	THR	conflict	UNP A0A3S8Q1D6
B	62	MET	VAL	conflict	UNP A0A3S8Q1D6
B	347	ILE	THR	conflict	UNP A0A3S8Q1D6
C	62	MET	VAL	conflict	UNP A0A3S8Q1D6
C	347	ILE	THR	conflict	UNP A0A3S8Q1D6

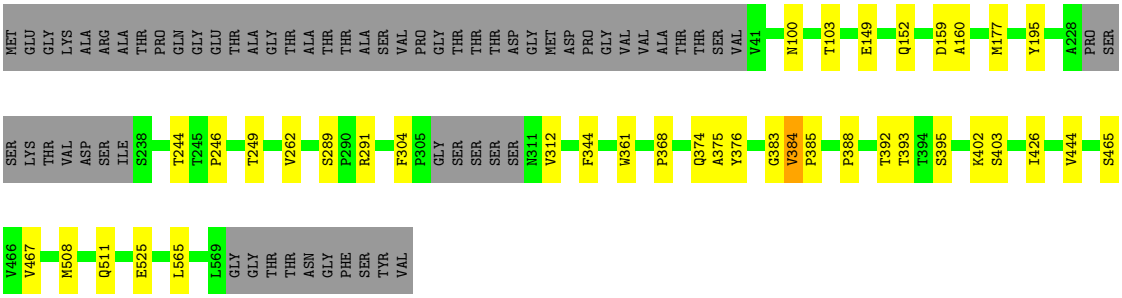
3 Residue-property plots (i)

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. 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. 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: Genome polyprotein

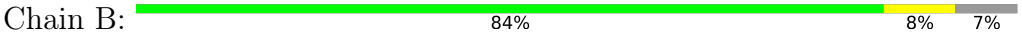
Chain A:

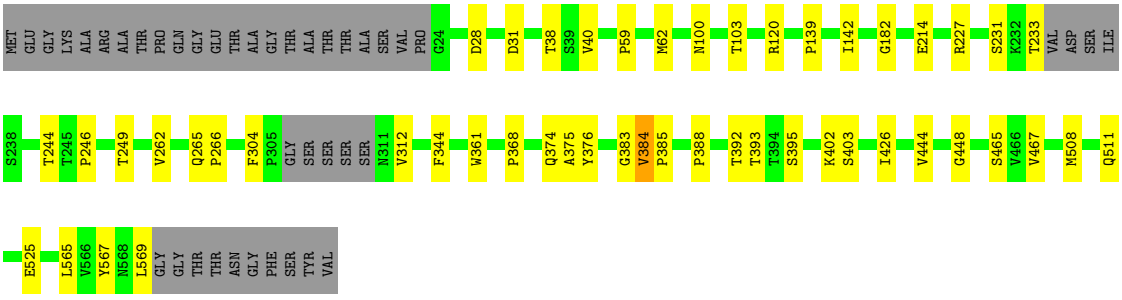




- Molecule 1: Genome polyprotein

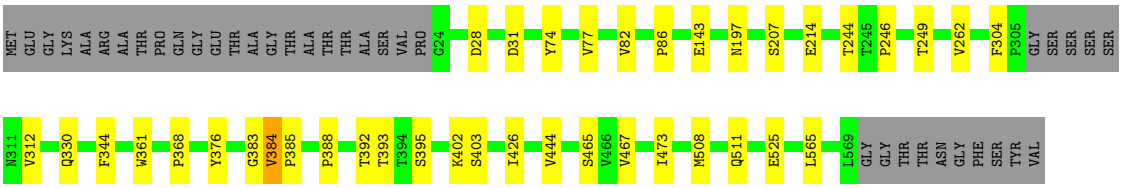
Chain B:





- Molecule 1: Genome polyprotein

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	21493	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 ($e^-/Å^2$)	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

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	0.25	0/3942	0.48	0/5412
1	B	0.25	0/4089	0.48	0/5615
1	C	0.25	0/4119	0.48	0/5658
All	All	0.25	0/12150	0.48	0/16685

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

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	3833	0	3692	21	0
1	B	3978	0	3834	33	0
1	C	4007	0	3864	29	0
All	All	11818	0	11390	78	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 (78) 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:B:448:GLY:H	1:C:330:GLN:HE22	1.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ILE:HG22	1:C:473:ILE:O	1.84	0.76
1:C:28:ASP:OD1	1:C:31:ASP:HB2	1.86	0.74
1:A:246:PRO:HA	1:A:249:THR:HG22	1.71	0.72
1:A:149:GLU:OE1	1:A:152:GLN:NE2	2.22	0.72
1:C:246:PRO:HA	1:C:249:THR:HG22	1.71	0.71
1:B:246:PRO:HA	1:B:249:THR:HG22	1.71	0.70
1:B:59:PRO:HB2	1:B:62:MET:HG3	1.76	0.68
1:C:392:THR:HA	1:C:444:VAL:HG22	1.79	0.65
1:B:448:GLY:N	1:C:330:GLN:HE22	1.95	0.64
1:A:392:THR:HA	1:A:444:VAL:HG22	1.79	0.63
1:B:392:THR:HA	1:B:444:VAL:HG22	1.79	0.63
1:B:448:GLY:HA2	1:C:330:GLN:NE2	2.16	0.60
1:B:244:THR:HG22	1:B:246:PRO:HD2	1.84	0.59
1:C:244:THR:HG22	1:C:246:PRO:HD2	1.84	0.59
1:A:244:THR:HG22	1:A:246:PRO:HD2	1.84	0.58
1:B:227:ARG:NH1	1:B:231:SER:OG	2.37	0.58
1:C:384:VAL:HG13	1:C:388:PRO:HA	1.87	0.57
1:C:473:ILE:O	1:C:473:ILE:CG2	2.52	0.57
1:B:384:VAL:HG13	1:B:388:PRO:HA	1.86	0.57
1:A:384:VAL:HG13	1:A:388:PRO:HA	1.86	0.56
1:C:74:TYR:HE1	1:C:77:VAL:HG23	1.69	0.56
1:A:384:VAL:N	1:A:385:PRO:HD3	2.21	0.56
1:C:384:VAL:N	1:C:385:PRO:HD3	2.21	0.55
1:B:384:VAL:N	1:B:385:PRO:HD3	2.21	0.55
1:C:74:TYR:HA	1:C:214:GLU:HG2	1.91	0.52
1:A:525:GLU:HB2	1:A:565:LEU:HB3	1.91	0.52
1:C:525:GLU:HB2	1:C:565:LEU:HB3	1.91	0.51
1:B:393:THR:HG22	1:B:395:SER:H	1.77	0.50
1:B:525:GLU:HB2	1:B:565:LEU:HB3	1.91	0.50
1:C:393:THR:HG22	1:C:395:SER:H	1.77	0.49
1:A:393:THR:HG22	1:A:395:SER:H	1.77	0.49
1:C:383:GLY:C	1:C:385:PRO:HD3	2.33	0.49
1:B:38:THR:HG22	1:B:40:VAL:HG22	1.95	0.49
1:A:383:GLY:C	1:A:385:PRO:HD3	2.33	0.49
1:B:383:GLY:C	1:B:385:PRO:HD3	2.33	0.48
1:B:448:GLY:N	1:C:330:GLN:NE2	2.61	0.48
1:C:344:PHE:O	1:C:402:LYS:NZ	2.43	0.48
1:B:376:TYR:HA	1:B:403:SER:HA	1.97	0.47
1:B:426:ILE:HD12	1:B:467:VAL:HG11	1.97	0.47
1:B:344:PHE:O	1:B:402:LYS:NZ	2.42	0.47
1:A:508:MET:HB2	1:A:511:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:MET:HB2	1:C:511:GLN:OE1	2.16	0.46
1:A:159:ASP:OD1	1:A:160:ALA:N	2.49	0.46
1:B:120:ARG:NH2	1:B:214:GLU:OE1	2.42	0.46
1:A:376:TYR:HA	1:A:403:SER:HA	1.96	0.46
1:C:376:TYR:HA	1:C:403:SER:HA	1.97	0.46
1:A:426:ILE:HD12	1:A:467:VAL:HG11	1.97	0.46
1:B:182:GLY:HA2	1:B:233:THR:HB	1.98	0.46
1:C:28:ASP:OD1	1:C:31:ASP:CB	2.59	0.46
1:B:100:ASN:HB3	1:B:103:THR:OG1	2.16	0.45
1:B:508:MET:HB2	1:B:511:GLN:OE1	2.15	0.45
1:B:139:PRO:HG2	1:B:142:ILE:HD12	1.98	0.45
1:C:86:PRO:HD3	1:C:197:ASN:OD1	2.17	0.45
1:C:426:ILE:HD12	1:C:467:VAL:HG11	1.97	0.45
1:B:448:GLY:CA	1:C:330:GLN:NE2	2.80	0.45
1:B:38:THR:HG22	1:B:40:VAL:H	1.83	0.44
1:A:344:PHE:O	1:A:402:LYS:NZ	2.43	0.43
1:A:361:TRP:HA	1:A:368:PRO:HA	2.00	0.43
1:A:304:PHE:HD2	1:A:312:VAL:HG21	1.84	0.43
1:A:262:VAL:HG22	1:A:465:SER:HA	2.00	0.43
1:C:361:TRP:HA	1:C:368:PRO:HA	2.00	0.43
1:B:361:TRP:HA	1:B:368:PRO:HA	2.00	0.43
1:C:262:VAL:HG22	1:C:465:SER:HA	2.01	0.42
1:B:304:PHE:HD2	1:B:312:VAL:HG21	1.83	0.42
1:B:262:VAL:HG22	1:B:465:SER:HA	2.01	0.41
1:C:304:PHE:HD2	1:C:312:VAL:HG21	1.84	0.41
1:C:82:VAL:HG22	1:C:207:SER:HB2	2.02	0.41
1:C:384:VAL:N	1:C:385:PRO:CD	2.84	0.41
1:A:289:SER:O	1:A:291:ARG:N	2.51	0.41
1:B:28:ASP:OD1	1:B:31:ASP:HB2	2.21	0.41
1:B:384:VAL:N	1:B:385:PRO:CD	2.84	0.41
1:A:100:ASN:HB3	1:A:103:THR:OG1	2.20	0.41
1:A:384:VAL:N	1:A:385:PRO:CD	2.84	0.41
1:B:265:GLN:NE2	1:B:266:PRO:O	2.50	0.40
1:B:567:TYR:HE1	1:B:569:LEU:HD22	1.86	0.40
1:A:374:GLN:HG3	1:A:375:ALA:H	1.87	0.40
1:B:374:GLN:HG3	1:B:375:ALA:H	1.87	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	509/579 (88%)	500 (98%)	8 (2%)	1 (0%)	44	54
1	B	531/579 (92%)	524 (99%)	6 (1%)	1 (0%)	44	54
1	C	537/579 (93%)	528 (98%)	8 (2%)	1 (0%)	44	54
All	All	1577/1737 (91%)	1552 (98%)	22 (1%)	3 (0%)	45	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	VAL
1	B	384	VAL
1	C	384	VAL

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	412/460 (90%)	410 (100%)	2 (0%)	86	92
1	B	430/460 (94%)	430 (100%)	0	100	100
1	C	434/460 (94%)	433 (100%)	1 (0%)	92	95
All	All	1276/1380 (92%)	1273 (100%)	3 (0%)	91	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	MET
1	A	195	TYR
1	C	143	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	C	330	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 oligosaccharides 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.