



Full wwPDB EM Validation Report ⓘ

Mar 8, 2025 – 06:03 am GMT

PDB ID : 9GJT
EMDB ID : EMD-51402
Title : Structure of Nipah Virus RNA Polymerase Complex - Apo state
Authors : Sala, F.; Ditter, K.; Dybkov, O.; Urlaub, H.; Hillen, H.S.
Deposited on : 2024-08-22
Resolution : 2.60 Å(reported)
Based on initial model : .

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) : 2.41

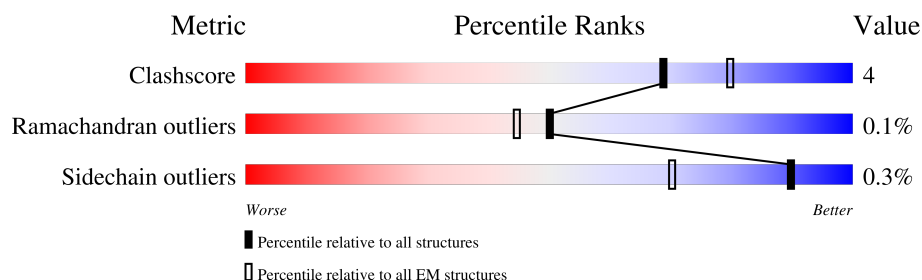
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	709	 24% . 72%
1	C	709	 14% . 85%
1	D	709	 13% . 85%
1	E	709	 13% . 85%
2	A	2246	 50% 5% 45%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14017 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	105	Total	C	N	O	S	0	0
			839	531	138	163	7		
1	D	103	Total	C	N	O	S	0	0
			818	516	135	160	7		
1	E	104	Total	C	N	O	S	0	0
			827	522	137	161	7		
1	B	196	Total	C	N	O	S	0	0
			1572	982	264	318	8		

- Molecule 2 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1233	Total	C	N	O	S	0	0
			9959	6352	1701	1840	66		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q997F0
A	0	ASN	-	expression tag	UNP Q997F0
A	1	ALA	-	expression tag	UNP Q997F0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	591312	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 ($e^-/\text{\AA}^2$)	48.94	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	B	0.24	0/1591	0.48	0/2147
1	C	0.25	0/853	0.45	0/1153
1	D	0.26	0/831	0.44	0/1124
1	E	0.24	0/840	0.43	0/1135
2	A	0.26	0/10165	0.50	0/13738
All	All	0.26	0/14280	0.49	0/19297

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	B	1572	0	1558	20	0
1	C	839	0	839	7	0
1	D	818	0	817	11	0
1	E	827	0	830	11	0
2	A	9959	0	9982	69	0
3	A	2	0	0	0	0
All	All	14017	0	14026	99	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 (99) 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:532:ARG:NH1	1:E:530:ASP:OD1	2.19	0.75
2:A:53:ASN:ND2	2:A:490:GLU:O	2.20	0.75
2:A:898:ASP:O	2:A:1368:ARG:NH1	2.20	0.74
2:A:881:GLU:N	2:A:881:GLU:OE1	2.24	0.71
1:D:489:PHE:O	1:D:493:THR:OG1	2.06	0.71
2:A:378:ARG:NH2	2:A:787:ASP:O	2.27	0.67
2:A:329:THR:O	2:A:334:ARG:NH2	2.28	0.66
1:B:648:ASN:OD1	1:B:650:SER:OG	2.09	0.66
2:A:1200:ARG:NH1	2:A:1217:GLU:OE2	2.28	0.66
2:A:82:GLU:OE1	2:A:225:LYS:NZ	2.30	0.64
2:A:339:ASP:OD2	1:B:665:LYS:NZ	2.23	0.64
2:A:867:ARG:NH2	1:B:640:PRO:O	2.30	0.64
1:C:543:ILE:HG23	1:B:546:ILE:HD11	1.79	0.63
2:A:90:GLU:N	2:A:90:GLU:OE1	2.32	0.61
2:A:1426:ASP:OD1	2:A:1427:ASN:N	2.34	0.61
2:A:418:LEU:HD22	2:A:453:ILE:HD11	1.83	0.61
2:A:999:PHE:HE1	2:A:1173:LEU:HD22	1.66	0.60
1:E:532:ARG:NH1	1:B:530:ASP:OD1	2.34	0.60
2:A:999:PHE:CE1	2:A:1173:LEU:HD22	2.38	0.59
2:A:1041:MET:HG3	2:A:1186:ILE:HG21	1.84	0.59
2:A:26:LEU:HD22	2:A:234:MET:CE	2.32	0.59
2:A:924:ARG:NH2	2:A:997:GLY:O	2.35	0.58
2:A:357:PHE:CE1	2:A:895:ILE:HD11	2.39	0.58
1:D:560:THR:OG1	1:E:561:ASN:OD1	2.19	0.57
2:A:275:LEU:HD11	2:A:337:PHE:CZ	2.39	0.57
1:C:523:SER:OG	1:B:525:LYS:NZ	2.32	0.57
2:A:357:PHE:CZ	2:A:895:ILE:HD11	2.39	0.57
2:A:183:VAL:CG2	2:A:199:ILE:HD12	2.34	0.57
2:A:471:MET:HA	2:A:506:VAL:HG12	1.86	0.56
1:B:656:ALA:N	1:B:691:ASP:OD1	2.39	0.56
2:A:1194:ASP:OD1	2:A:1197:ARG:NH2	2.38	0.56
2:A:243:GLU:OE2	2:A:954:LYS:NZ	2.39	0.56
2:A:1432:GLU:N	2:A:1432:GLU:OE1	2.38	0.56
1:C:517:LEU:HD21	1:B:500:ALA:HA	1.87	0.55
1:B:579:PRO:O	1:B:594:LEU:N	2.39	0.55
2:A:116:LYS:HE3	2:A:983:LEU:HD11	1.88	0.55
2:A:1328:ASP:OD1	2:A:1329:LEU:N	2.40	0.54
1:C:574:MET:O	1:B:598:ILE:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:SER:O	1:B:663:VAL:HG23	2.08	0.54
2:A:521:LEU:HD21	2:A:566:ILE:HG21	1.90	0.54
1:D:536:ILE:O	1:D:540:VAL:HG22	2.08	0.54
2:A:1017:THR:HG21	2:A:1218:VAL:O	2.09	0.53
2:A:1223:GLU:O	2:A:1425:LYS:NZ	2.39	0.53
2:A:328:PHE:O	2:A:334:ARG:NE	2.42	0.53
1:C:516:VAL:O	1:C:520:VAL:HG23	2.09	0.53
1:C:560:THR:HG23	1:D:564:LEU:HD11	1.90	0.52
2:A:575:VAL:HG21	2:A:742:LEU:HD22	1.91	0.52
1:E:512:CYS:O	1:E:516:VAL:HG23	2.09	0.52
2:A:484:ASP:OD2	2:A:778:HIS:ND1	2.42	0.52
2:A:1217:GLU:N	2:A:1217:GLU:OE1	2.43	0.51
1:B:661:ARG:NH2	1:B:685:LEU:O	2.43	0.51
2:A:473:ASP:OD1	2:A:504:ARG:NE	2.40	0.50
1:E:560:THR:HG23	1:B:564:LEU:CD1	2.42	0.50
1:B:658:ASP:OD1	1:B:659:SER:N	2.44	0.50
2:A:264:ARG:NH1	2:A:344:ILE:O	2.43	0.49
2:A:1252:PRO:O	2:A:1255:SER:OG	2.30	0.49
2:A:1238:ILE:HG22	2:A:1243:ASN:HB3	1.94	0.49
2:A:733:GLU:OE1	2:A:733:GLU:N	2.42	0.49
2:A:849:LYS:NZ	1:B:706:ASP:O	2.44	0.49
1:B:704:ILE:HG13	1:B:709:ILE:HD12	1.95	0.49
2:A:715:VAL:HG11	2:A:851:LYS:HB3	1.94	0.49
1:B:690:ASN:OD1	1:B:691:ASP:N	2.45	0.49
1:E:560:THR:HG23	1:B:564:LEU:HD11	1.94	0.49
2:A:1235:GLU:OE1	2:A:1235:GLU:N	2.43	0.48
2:A:970:THR:HG21	2:A:1163:SER:O	2.13	0.48
1:D:488:PHE:HZ	1:E:524:ILE:HG21	1.79	0.48
2:A:1170:PHE:O	2:A:1174:ASN:ND2	2.46	0.47
2:A:1193:VAL:HG13	2:A:1217:GLU:HB3	1.97	0.47
1:D:479:MET:O	1:D:483:ASP:N	2.49	0.46
1:C:530:ASP:O	1:C:534:ASN:ND2	2.49	0.46
2:A:817:SER:O	2:A:821:THR:HG22	2.15	0.46
2:A:725:LYS:O	2:A:729:ASN:ND2	2.49	0.46
2:A:1061:ASN:ND2	2:A:1206:GLU:OE2	2.48	0.45
2:A:1298:ARG:O	2:A:1302:VAL:HG23	2.16	0.45
2:A:350:ILE:HD11	2:A:1258:ASP:HA	1.99	0.45
2:A:280:GLY:O	2:A:283:ILE:HG22	2.17	0.45
2:A:176:ILE:HD11	2:A:208:ILE:HD13	1.99	0.44
2:A:491:VAL:HG21	2:A:769:PRO:O	2.17	0.44
2:A:948:TYR:CE2	2:A:952:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:249:GLU:OE2	2:A:253:LYS:NZ	2.29	0.44
2:A:575:VAL:HG21	2:A:742:LEU:CD2	2.48	0.44
2:A:130:GLN:NE2	2:A:151:CYS:SG	2.88	0.43
1:E:552:SER:O	1:E:556:VAL:HG23	2.18	0.43
2:A:300:LEU:HD11	1:B:667:LEU:HG	2.00	0.43
2:A:1014:ASP:HB3	2:A:1017:THR:HG22	2.01	0.43
1:D:532:ARG:NH1	1:E:530:ASP:O	2.39	0.42
2:A:346:ASN:ND2	1:B:670:THR:OG1	2.46	0.42
2:A:26:LEU:HD22	2:A:234:MET:HE1	2.02	0.41
2:A:490:GLU:OE1	2:A:490:GLU:N	2.49	0.41
2:A:23:SER:HA	2:A:367:ILE:HD11	2.02	0.41
1:D:556:VAL:HG11	1:E:557:LEU:HB3	2.02	0.41
2:A:302:ASP:OD1	2:A:303:GLU:N	2.54	0.41
2:A:773:PRO:HB3	2:A:789:ILE:HD11	2.03	0.41
2:A:259:GLN:HG2	2:A:262:ILE:HD12	2.03	0.41
2:A:418:LEU:HD21	2:A:455:PHE:CE1	2.56	0.41
1:D:491:HIS:ND1	1:D:492:ASP:OD1	2.52	0.40
2:A:290:ILE:O	2:A:294:VAL:HG23	2.21	0.40
2:A:1377:LEU:HD21	2:A:1395:ALA:HB3	2.03	0.40
1:D:532:ARG:NH2	1:E:534:ASN:OD1	2.49	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	B	190/709 (27%)	188 (99%)	2 (1%)	0	100	100
1	C	103/709 (14%)	101 (98%)	2 (2%)	0	100	100
1	D	101/709 (14%)	100 (99%)	1 (1%)	0	100	100
1	E	102/709 (14%)	101 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	1219/2246 (54%)	1191 (98%)	27 (2%)	1 (0%)	48 71
All	All	1715/5082 (34%)	1681 (98%)	33 (2%)	1 (0%)	50 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	789	ILE

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 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	B	182/625 (29%)	181 (100%)	1 (0%)	86 95
1	C	98/625 (16%)	98 (100%)	0	100 100
1	D	96/625 (15%)	95 (99%)	1 (1%)	73 88
1	E	97/625 (16%)	97 (100%)	0	100 100
2	A	1112/2047 (54%)	1109 (100%)	3 (0%)	91 97
All	All	1585/4547 (35%)	1580 (100%)	5 (0%)	90 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	512	CYS
2	A	464	ASP
2	A	1112	ARG
2	A	1314	TRP
1	B	530	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	522	ASN

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Mol	Chain	Res	Type
1	C	534	ASN
1	D	499	HIS
1	D	502	HIS
1	D	539	GLN
2	A	130	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.