

Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2022 – 02:09 PM JST

PDB ID	:	7F0S
Title	:	A crystal structure of alphavirus nonstructural protein 4 (nsP4) reveals an
		intrinsically 1dynamic RNA-dependent RNA polymerase
Authors	:	Tan, Y.B.; Luo, D.
Deposited on	:	2021-06-06
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	А	502	8%	19%	17%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3109 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 RNA-directed RNA polymerase nsP4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	419	Total 3108	C 1978	N 529	O 579	S 22	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	192	ALA	GLN	engineered mutation	UNP P13888
А	196	ALA	GLN	engineered mutation	UNP P13888

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total O 1 1	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: RNA-directed RNA polymerase nsP4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	64.84Å 68.35Å 99.65Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	27.13 - 2.60	Depositor
Resolution (A)	47.04 - 2.30	EDS
% Data completeness	99.7 (27.13-2.60)	Depositor
(in resolution range)	85.8 (47.04-2.30)	EDS
R_{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	-0.04 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
P. P.	0.265 , 0.288	Depositor
Λ, Λ_{free}	0.266 , 0.288	DCC
R_{free} test set	1005 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	65.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 98.1	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3109	wwPDB-VP
Average B, all atoms $(Å^2)$	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.32	0/3115	0.58	2/4237~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	514	LYS	CD-CE-NZ	-6.35	97.09	111.70
1	А	526	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	514	LYS	Peptide

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	А	3108	0	3013	73	2
2	А	1	0	0	1	0
All	All	3109	0	3013	73	2

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 12.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:506:CYS:O	1:A:521:ARG:NH2	2.22	0.72
1:A:497:THR:HB	1:A:500:GLU:HB2	1.75	0.69
1:A:557:TRP:HB2	1:A:566:LEU:HD13	1.74	0.68
1:A:113:ASP:OD1	1:A:114:SER:N	2.29	0.66
1:A:497:THR:H	1:A:501:LYS:HB2	1.61	0.65
1:A:320:THR:HG22	1:A:427:MET:HB2	1.79	0.64
1:A:253:ILE:HD12	1:A:281:VAL:HG21	1.83	0.60
1:A:442:LEU:HA	1:A:445:VAL:HG12	1.82	0.60
1:A:267:ALA:O	1:A:271:LYS:HB2	2.03	0.59
1:A:276:VAL:HG13	1:A:279:GLN:HB2	1.83	0.59
1:A:327[B]:HIS:NE2	1:A:430:SER:O	2.37	0.58
1:A:283:MET:HA	1:A:286:PHE:CE2	2.39	0.58
1:A:191:PHE:HB3	1:A:412:THR:HA	1.85	0.58
1:A:326:ILE:HD11	1:A:400:LEU:HD22	1.86	0.57
1:A:286:PHE:C	1:A:312:ILE:HD12	2.24	0.57
1:A:191:PHE:HD2	1:A:412:THR:HG22	1.70	0.56
1:A:270:ALA:HB1	1:A:275:LEU:HB2	1.86	0.56
1:A:508:GLY:HA2	1:A:524:ASP:HB2	1.87	0.56
1:A:114:SER:HB3	1:A:120:VAL:HG11	1.88	0.56
1:A:248:ILE:HG23	1:A:252:ASN:HB2	1.88	0.55
1:A:535:PRO:HA	1:A:599:LEU:HD23	1.88	0.55
1:A:215:LEU:O	1:A:217:THR:N	2.41	0.54
1:A:497:THR:N	1:A:501:LYS:HB2	2.22	0.54
1:A:474:ARG:NH1	1:A:496:ALA:O	2.39	0.54
1:A:268:LEU:O	1:A:272:THR:OG1	2.14	0.52
1:A:513:ASP:OD2	1:A:559:ARG:NH1	2.42	0.52
1:A:222:VAL:O	1:A:225:VAL:HG22	2.10	0.51
1:A:190:PRO:HA	1:A:415:HIS:HA	1.90	0.51
1:A:327[B]:HIS:CE1	1:A:434:LEU:HD22	2.45	0.51
1:A:248:ILE:HB	1:A:322:TYR:CD1	2.46	0.51
1:A:316:GLU:N	1:A:317:PRO:HD2	2.26	0.50
1:A:316:GLU:H	1:A:317:PRO:HD2	1.76	0.50

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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:258:THR:HG22	1:A:263:PRO:HA	1.93	0.49
1:A:564:SER:O	1:A:567:GLU:HG2	2.12	0.49
1:A:332:ARG:HD2	1:A:332:ARG:C	2.33	0.49
1:A:416:LEU:HD12	1:A:422:PHE:CE2	2.49	0.47
1:A:117:ASN:OD1	1:A:119:GLU:N	2.44	0.47
1:A:248:ILE:HG23	1:A:252:ASN:CB	2.45	0.46
1:A:343:HIS:HE1	2:A:1501:HOH:O	1.98	0.46
1:A:250:THR:O	1:A:254:THR:HG23	2.15	0.46
1:A:327[B]:HIS:CE1	1:A:434:LEU:HB3	2.51	0.45
1:A:268:LEU:HA	1:A:271:LYS:HB3	1.99	0.45
1:A:450:VAL:HG12	1:A:451:LEU:HD12	1.99	0.45
1:A:118:PRO:HB3	1:A:594:LYS:HD3	2.00	0.44
1:A:172:UNK:HA	1:A:433:PHE:CE2	2.53	0.44
1:A:276:VAL:HG13	1:A:279:GLN:CB	2.48	0.44
1:A:431:GLY:HA2	1:A:434:LEU:CD2	2.48	0.44
1:A:374:SER:HB2	1:A:490:GLU:OE1	2.18	0.44
1:A:221:ALA:O	1:A:225:VAL:HG13	2.18	0.43
1:A:276:VAL:HG22	1:A:279:GLN:HG3	2.00	0.43
1:A:596:PHE:HA	1:A:599:LEU:HD13	1.98	0.43
1:A:329:GLU:HG3	1:A:333:ARG:HD2	2.00	0.43
1:A:496:ALA:HA	1:A:501:LYS:CB	2.49	0.43
1:A:267:ALA:O	1:A:271:LYS:CB	2.66	0.42
1:A:253:ILE:CD1	1:A:281:VAL:HG21	2.49	0.42
1:A:327[B]:HIS:HE2	1:A:430:SER:C	2.22	0.42
1:A:512:TYR:HA	1:A:519:ALA:HA	2.02	0.42
1:A:191:PHE:CD2	1:A:412:THR:HG22	2.52	0.42
1:A:276:VAL:O	1:A:279:GLN:HB2	2.20	0.42
1:A:248:ILE:HB	1:A:322:TYR:CE1	2.55	0.42
1:A:286:PHE:CZ	1:A:322:TYR:CD2	3.08	0.41
1:A:372:ILE:HB	1:A:466:ASP:HB2	2.01	0.41
1:A:552:ASP:OD1	1:A:553:GLU:N	2.53	0.41
1:A:287:VAL:N	1:A:312:ILE:HD12	2.36	0.41
1:A:449:ARG:HA	1:A:449:ARG:HD2	1.88	0.41
1:A:514:LYS:HD2	1:A:514:LYS:O	2.20	0.41
1:A:523:ALA:HB3	1:A:553:GLU:OE1	2.20	0.41
1:A:478:LEU:HD12	1:A:478:LEU:HA	1.73	0.41
1:A:524:ASP:OD2	1:A:526:LEU:HG	2.21	0.41
1:A:544:GLU:HB2	1:A:549:ALA:HB2	2.02	0.41
1:A:270:ALA:CB	1:A:275:LEU:HB2	2.50	0.41
1:A:382:SER:O	1:A:386:THR:OG1	2.28	0.41
1:A:194:THR:HG21	1:A:439:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASP:OD2	1:A:449:ARG:NH2[2_655]	2.17	0.03
1:A:114:SER:OG	1:A:415:HIS:O[4_446]	2.17	0.03

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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	А	399/502~(80%)	369~(92%)	30 (8%)	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 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	А	316/380~(83%)	315 (100%)	1 (0%)	92 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	514	LYS

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



Mol	Chain	Res	Type
1	A	239	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 monosaccharides 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, 95^{th} 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	А	410/502~(81%)	0.58	42 (10%) 6 4	60, 108, 161, 226	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	120	VAL	12.6
1	А	547	ARG	9.7
1	А	599	LEU	8.0
1	А	259	ARG	7.6
1	А	536	LEU	7.4
1	А	537	PRO	6.9
1	А	186	ALA	6.4
1	А	541	THR	5.0
1	А	538	ALA	4.8
1	А	600	ARG	4.8
1	А	115	LEU	4.3
1	А	595	ASN	4.2
1	А	132	ASN	3.9
1	А	422	PHE	3.9
1	А	555	ASP	3.7
1	А	315	ALA	3.6
1	А	585	ALA	3.5
1	А	290	MET	3.4
1	А	558	ALA	3.2
1	А	207	CYS	3.1
1	А	268	LEU	2.9
1	А	488	ASN	2.7
1	А	586	MET	2.6
1	А	557	TRP	2.6
1	А	487	VAL	2.6
1	А	116	GLN	2.6
1	А	378	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	А	497	THR	2.4
1	А	572	SER	2.4
1	А	412	THR	2.4
1	А	347	ASP	2.3
1	А	475	SER	2.3
1	А	328	ARG	2.3
1	А	119	GLU	2.2
1	А	344	THR	2.2
1	А	479	MET	2.2
1	А	418	THR	2.2
1	А	546	ARG	2.1
1	А	192	ALA	2.1
1	А	112	GLU	2.1
1	А	478	LEU	2.1
1	А	291	LYS	2.0

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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 monosaccharides 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.

