



## wwPDB EM Validation Summary Report ⓘ

May 5, 2026 – 06:18 PM JST

PDB ID : 9VXV / pdb\_00009vxv  
EMDB ID : EMD-65442  
Title : Cryo-EM Structure of Nipah Virus Polymerase in complex with ERDRP-0519  
Authors : Xue, L.; Gui, J.; Chang, T.; Pan, H.; Xiong, X.  
Deposited on : 2025-07-20  
Resolution : 2.66 Å(reported)

This is a wwPDB EM Validation Summary 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>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

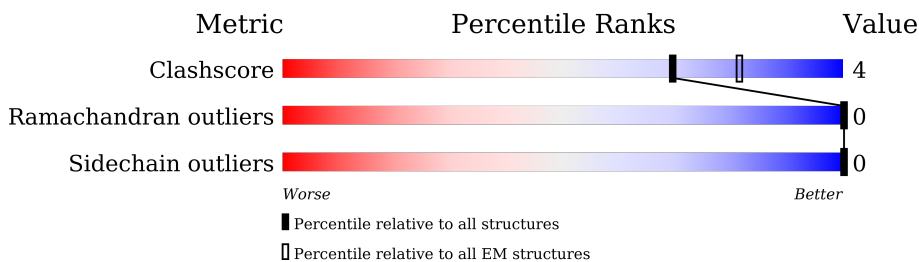
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.66 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	2244	
2	B	709	
2	C	709	
2	D	709	
2	E	709	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13295 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1315	Total	C	N	O	S	0	0
			10584	6747	1811	1959	67		

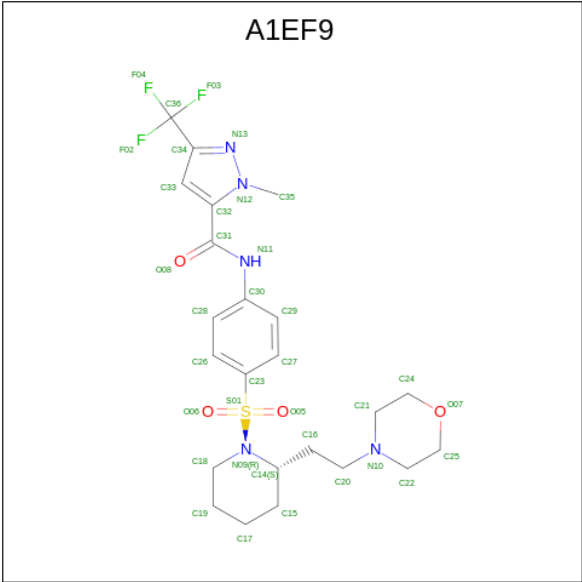
- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	151	Total	C	N	O	S	1	0
			1215	761	207	242	5		
2	C	55	Total	C	N	O	S	0	0
			437	278	75	80	4		
2	D	71	Total	C	N	O	S	0	0
			558	351	101	102	4		
2	E	59	Total	C	N	O	S	0	0
			463	294	81	84	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 2-methyl- {N}-[4-[(2 {S})-2-(2-morpholin-4-ylethyl)piperidin-1-yl]sulfonylphenyl]-5-(trifluoromethyl)pyrazole-3-carboxamide (CCD ID: A1EF9) (formula: C<sub>23</sub>H<sub>30</sub>F<sub>3</sub>N<sub>5</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).

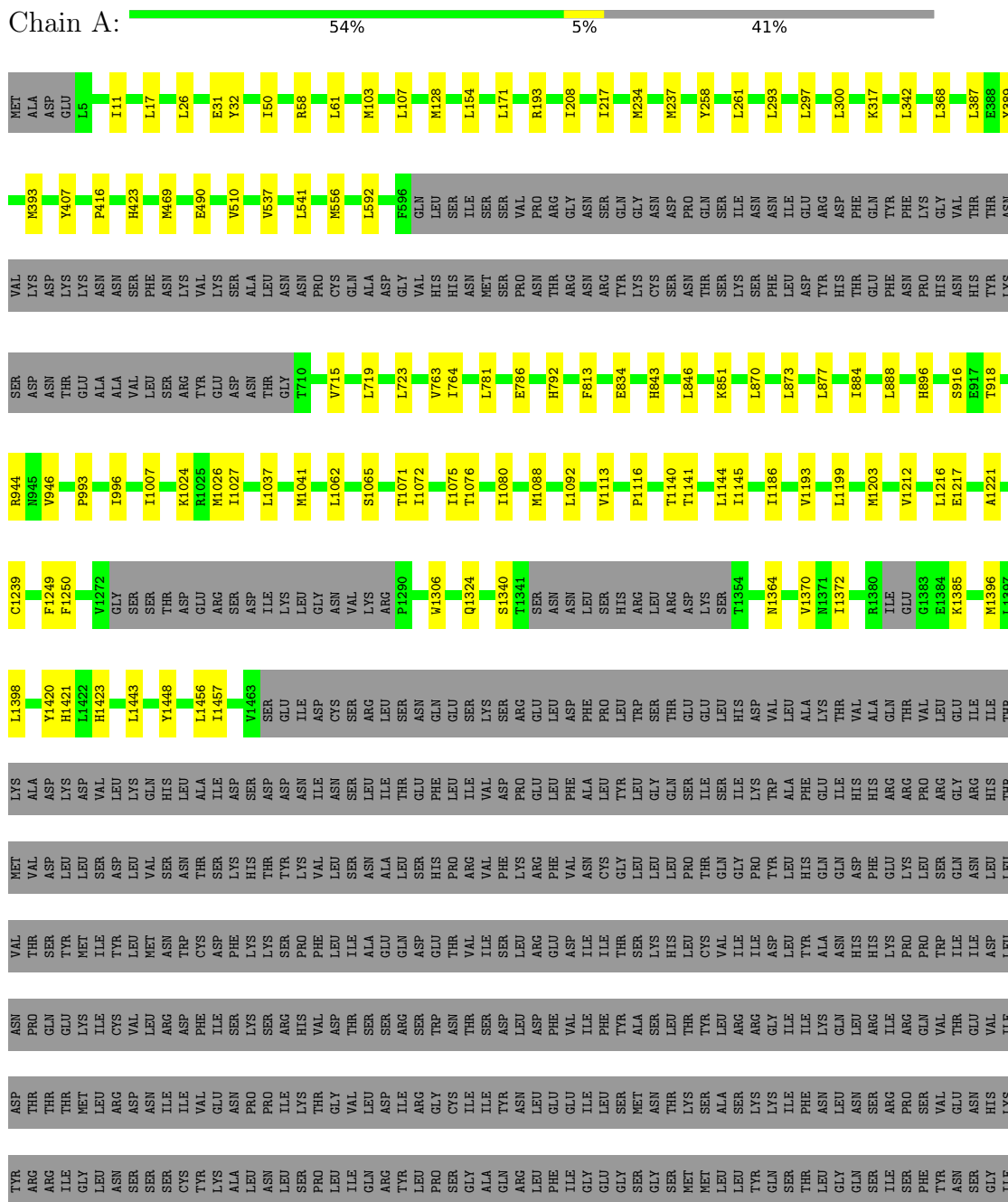


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	36	23	3	5	4	1	0

### 3 Residue-property plots

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: RNA-directed RNA polymerase L



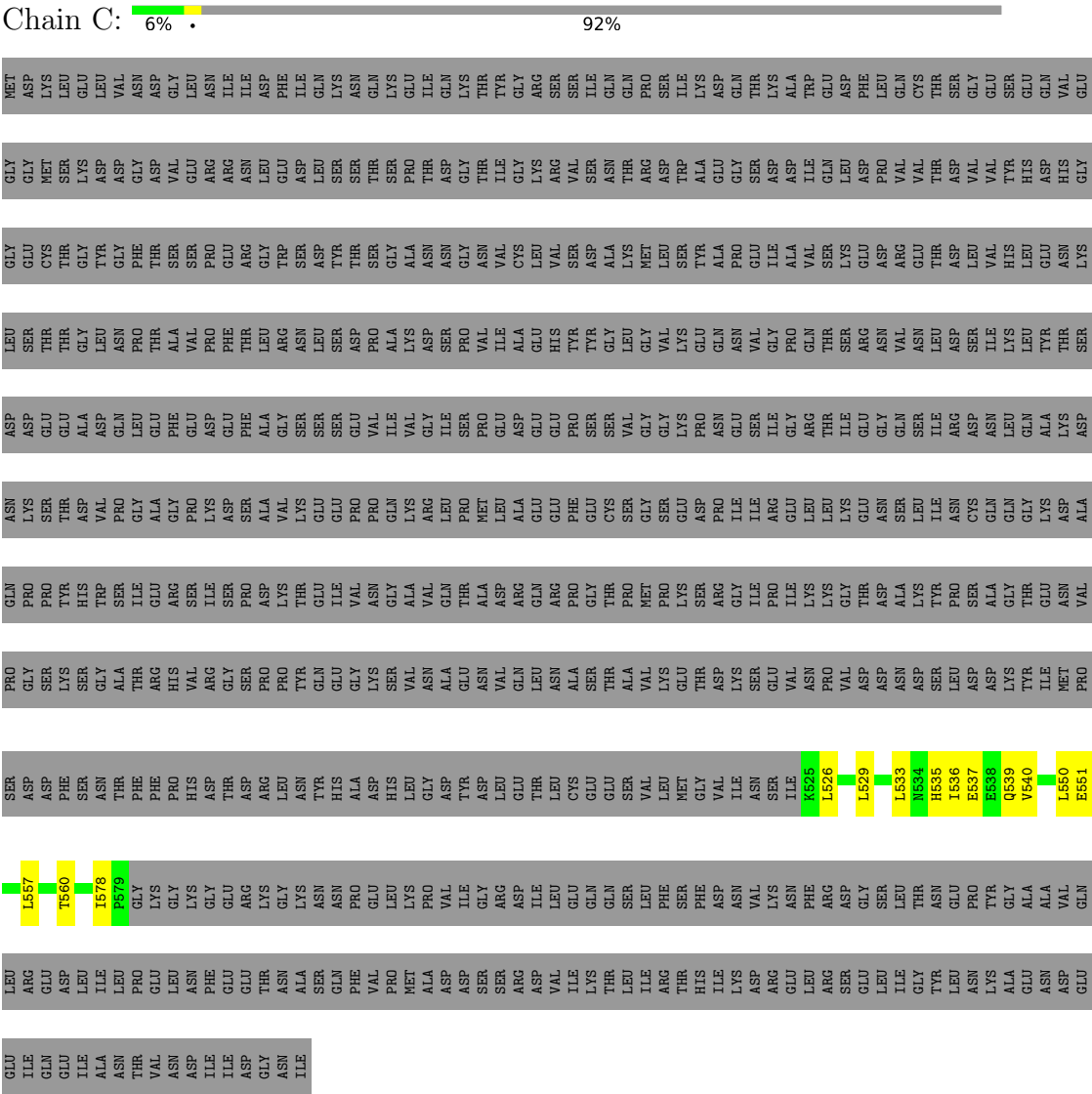
ARG	LEU	ASP	SER	PHE	THR	ASP
GLU	ILE	ILE	VAL	VAL	ALA	GLY
VAL	LYS	GLY	ILE	MET	GLY	ASP
LYS	PHE	SER	PHE	TYR	ARG	TYR
ILE	LYS	ASP	LYS	ARG	SER	ILE
TRP	ASP	ILE	ILE	TYR	ILE	PRO
TRP	THR	ASN	LYS	TYR	GLY	GLY
LYS	LYS	THR	ASN	PHE	LEU	GLN
ILE	SER	LEU	ASN	VAL	VAL	ARG
ILE	SER	ARG	GLN	LEU	HIS	GLU
GLY	GLU	ASP	SER	VAL	SER	LEU
TYR	LEU	THR	LYS	LEU	ASP	LYS
ILE	TYR	ILE	GLN	VAL	LEU	LEU
ILE	HIS	ILE	PHE	CYS	MET	PHE
SER	ILE	ILE	HIS	CYS	GLU	GLY
ILE	LYS	MET	ASP	PRO	GLY	SER
	ASN	LEU	ASP	VAL	ILE	TYR
	ASN	ASN	LEU	TYR	ASP	SER
	ILE	GLU	LYS	SER	LYS	TYR
	ARG	ALA	LYS	SER	ASN	ILE
	ARG	MET	TYR	PRO	VAL	ALA
	LYS	ASN	ASP	ASN	GLU	GLU
	VAL	TYR	GLN	SER	GLY	GLU
	LEU	PHE	ILE	THR	ILE	ASP
	ILE	ASP	ASP	GLU	LEU	PRO
	LEU	ASP	GLN	VAL	VAL	SER
	LEU	ASN	PRO	TYR	GLU	LEU
	PHE	ARG	PHE	LEU	HIS	GLY
	ARG	SER	PHE	LEU	SER	GLY
	SER	PRO	VAL	CYS	HIS	LYS
	LYS	SER	PRO	LEU	LEU	LYS
	LEU	HIS	THR	GLN	ILE	LYS
	MET	THR	ILE	THR	ILE	LEU
	LYS	GLU	THR	VAL	ALA	VAL
	THR	PRO	SER	LYS	ILE	VAL
	LEU	TYR	ASP	THR	ASN	PRO
	PRO	PRO	GLU	ILE	VAL	LEU
	LYS	VAL	GLN	VAL	MET	PHE
	GLY	LEU	VAL	PRO	MET	ASN
	MET	GLU	LEU	PRO	GLY	GLY
	GLN	ARG	LEU	GLN	ASP	ARG
	ARG	THR	GLU	LYS	GLY	PRO
	GLU	ARG	ALA	VAL	LEU	GLU
	ARG	ILE	GLY	LEU	LEU	THR
	GLU	GLU	LEU	GLU	VAL	THR
	LYS	THR	LYS	HIS	SER	TRP
	ASN	ILE	LEU	SER	LYS	ILE
	GLY	MET	ASN	ASN	ILE	GLY
	PHE	ASN	GLY	LEU	ALA	ASN
	LYS	CYS	PRO	HIS	TYR	LEU
	GLU	VAL	GLU	ASP	THR	ASP
	VAL	THR	ILE	GLU	PRO	SER
	TRP	LYS	LEU	VAL	GLY	TYR
	ILE	LYS	LYS	ASN	PHE	GLU
	VAL	VAL	VAL	SER	PRO	TYR
	ASP	ILE	GLU	GLN	ILE	ILE
	LEU	VAL	ILE	GLY	SER	ILE
	ASN	TYR	SER	ILE	ARG	ASN
	SER	SER	THR	THR	LEU	ARG

- Molecule 2: Phosphoprotein

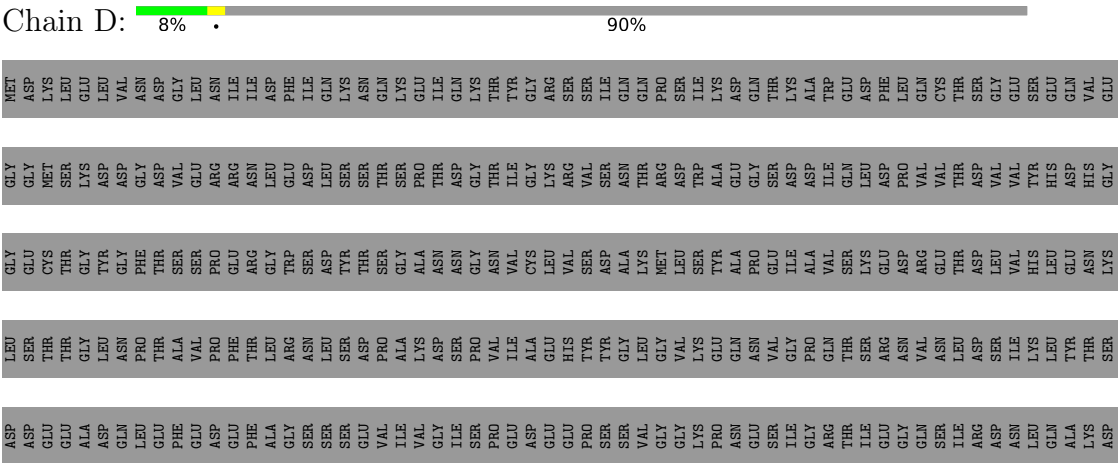
Chain B:  18% 2% 79%

1769	L564	SER	PRO	GLN	ASN	ASP	LEU	GLY	GLY	ASP	MET
		ASP	GLY	PRO	LYS	ASP	SER	SER	GLY	ASP	
	M575	PHE	LYS	TYR	THR	THR	THR	THR	THR	CYS	LYS
	1576	SER	SER	HIS	ASP	ALA	GLY	GLY	LYS	SER	LEU
		ASN	GLY	TRP	VAL	VAL	ASP	LEU	TYR	ASP	LEU
	P579	THR	ALA	SER	PRO	GLN	ASN	ASN	GLY	ASP	VAL
	GLY	PHE	THR	ILE	PRO	LEU	PRO	PRO	PHE	GLY	ASN
	LYS	PHE	ARG	GLU	ALA	GLY	THR	THR	THR	ASP	GLY
	GLY	PRO	HIS	ARG	GLY	GLY	ALA	ALA	SER	VAL	GLY
	LYS	VAL	VAL	SER	PRO	LYS	VAL	VAL	SER	GLU	ASN
	GLY	ARG	ILE	ILE	LYS	ASP	PRO	PRO	ARG	ASN	LEU
	GLU	THR	GLY	SER	ASP	GLU	GLU	PHE	GLU	ARG	ILE
	ARG	ASP	PRO	PRO	SER	PHE	THR	THR	THR	ASN	ILE
	LYS	ARG	PRO	ASP	ALA	ALA	GLY	GLY	GLY	LEU	ILE
	LYS	ASN	TYR	THR	LYS	SER	ASN	ASP	ASP	GLU	ASN
	ASN	TYR	GLN	THR	GLU	SER	LEU	LEU	SER	GLY	GLN
	ASN	HIS	GLY	ILE	GLU	SER	SER	SER	TYR	GLN	LYS
	PRO	ALA	GLY	VAL	PRO	GLU	ASP	ASP	THR	SER	ASN
	E593	HIS	LYS	VAL	ASN	PRO	VAL	PRO	THR	SER	GLN
	L594	HIS	SER	GLY	GLN	ILE	ALA	ALA	SER	THR	LYS
K595	LEU	VAL	ALA	LYS	VAL	VAL	LYS	ALA	PRO	GLU	
P596	GLY	ASN	VAL	ARG	GLY	ILE	ASP	ASN	THR	ILE	
	ASP	ALA	GLN	GLM	LEU	GLY	SER	ASN	ASP	GLM	
T602	TYR	GLU	THR	THR	PRO	SER	PRO	GLY	GLY	LYS	
	ASP	ASN	VAL	ARG	ALA	ASP	GLU	LEU	VAL	ARG	
S610	GLU	GLN	ASP	ALA	ALA	ASP	ALA	CYS	GLY	LYS	
PHE	THR	LEU	GLM	GLN	GLU	GLY	GLU	LEU	VAL	ARG	
ASN	LEU	ASN	ASN	ARG	GLU	GLY	GLU	THR	SER	SER	
VAL	CYS	ALA	PRO	PHE	THR	PRO	TYR	TYR	VAL	ILE	
LYS	GLU	SER	GLY	GLY	GLU	SER	GLY	ASP	SER	ILE	
ASN	GLU	THR	THR	CYS	SER	SER	GLY	ALA	ASN	GLN	
PHE	SER	ALA	PRO	SER	VAL	VAL	THR	THR	THR	GLN	
ARG	VAL	VAL	MET	GLY	GLY	GLY	GLY	ARG	ARG	PRO	
ASP	LEU	LYS	PRO	SER	SER	GLY	VAL	LEU	ASP	PRO	
GLY	GLY	THR	THR	LYS	GLU	LYS	LYS	TRP	ASP	ILE	
SER	GLY	GLU	GLU	SER	PRO	TYR	GLU	ALA	ALA	LYS	
LEU	VAL	VAL	ARG	ARG	ASN	GLN	ASN	GLY	GLY	GLN	
THR	ILE	LYS	LYS	ILE	GLU	PRO	ASN	PRO	GLY	ASN	
ASN	ASN	SER	SER	ILE	SER	VAL	ASN	VAL	SER	THR	
GLU	GLU	SER	GLU	ARG	ILE	GLY	GLY	ILE	ASP	ALA	
PRO	ILE	SER	VAL	PRO	ARG	ILE	GLY	GLY	ASP	ALA	
TYR	K525	GLY	ASN	LYS	THR	THR	SER	GLN	ILE	GLU	
ALA	L533	VAL	VAL	GLY	LYS	ILE	SER	LYS	LEU	PHE	
ALA	ALA	ASP	ASP	THR	GLN	GLY	GLY	GLU	ASP	LEU	
VAL	E537	VAL	ASP	ASP	ASN	GLY	GLY	ASN	PRO	THR	
	E538	ASP	ASN	SER	SER	GLN	GLN	VAL	GLN	CYS	
	Q539	ASP	LYS	LEU	LEU	ASN	ASN	VAL	VAL	THR	
	V540	SER	TYR	ILE	ILE	ILE	ILE	THR	THR	THR	
	K541	LEU	PRO	PRO	ASN	ASN	ASP	ASP	ASP	SER	
		ASP	ASP	SER	GLY	ARG	SER	LEU	VAL	GLY	
	ALA	ALA	VAL	THR	LYS	ILE	THR	GLY	VAL	THR	
	VAL	E537	ASP	ASP	ASN	GLY	GLY	GLY	ASP	THR	
	Q632	VAL	ASP	THR	GLN	ASN	ASN	ARG	VAL	GLY	
			ASP	LYS	ILE	GLN	ASN	ASP	VAL	GLY	
	T647	GLY	PRO	LYS	ILE	ILE	THR	THR	THR	SER	
		ALA	VAL	GLY	ASN	ASN	ASP	ASP	VAL	GLY	
	V653	VAL	ASP	SER	CYS	ASP	SER	SER	VAL	SER	
	P654	ASP	LYS	ALA	GLN	ASN	ILE	GLY	GLY	SER	
	1654	THR	GLY	GLN	GLY	LEU	LYS	HIS	THR	GLY	
		E551	ILE	GLU	LYS	ALA	THR	GLY	GLY	GLN	
	L667	THR	PRO	ASN	ASP	VAL	THR	LYS	VAL	GLY	
		V556	ASN	VAL	ALA	ASP	SER	LYS	THR	THR	

- Molecule 2: Phosphoprotein



● Molecule 2: Phosphoprotein





THR  
VAL  
ASN  
ASP  
ILE  
ILE  
ASP  
GLY  
ASN  
ILE

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4539359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k 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: A1EF9, 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	A	0.16	0/10803	0.31	0/14604
2	B	0.17	0/1227	0.40	0/1652
2	C	0.23	0/440	0.54	0/591
2	D	0.21	0/562	0.45	0/749
2	E	0.20	0/466	0.46	0/623
All	All	0.17	0/13498	0.34	0/18219

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	10584	0	10624	67	0
2	B	1215	0	1248	17	0
2	C	437	0	476	11	0
2	D	558	0	608	9	0
2	E	463	0	508	7	0
3	A	2	0	0	0	0
4	A	36	0	0	0	0
All	All	13295	0	13464	97	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.

The worst 5 of 97 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:A:1239:CYS:SG	1:A:1423:HIS:CE1	2.84	0.70
1:A:1249:PHE:HB2	1:A:1420:TYR:HB3	1.76	0.68
1:A:843:HIS:HB3	1:A:846:LEU:HD13	1.77	0.66
1:A:58:ARG:HH12	1:A:490:GLU:HG3	1.61	0.66
1:A:26:LEU:HD22	1:A:234:MET:HE1	1.78	0.65

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	1305/2244 (58%)	1259 (96%)	46 (4%)	0	100	100
2	B	146/709 (21%)	144 (99%)	2 (1%)	0	100	100
2	C	53/709 (8%)	52 (98%)	1 (2%)	0	100	100
2	D	69/709 (10%)	68 (99%)	1 (1%)	0	100	100
2	E	57/709 (8%)	56 (98%)	1 (2%)	0	100	100
All	All	1630/5080 (32%)	1579 (97%)	51 (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	1180/2046 (58%)	1180 (100%)	0	100	100
2	B	142/625 (23%)	142 (100%)	0	100	100
2	C	52/625 (8%)	52 (100%)	0	100	100
2	D	64/625 (10%)	64 (100%)	0	100	100
2	E	54/625 (9%)	54 (100%)	0	100	100
All	All	1492/4546 (33%)	1492 (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. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	770	ASN
2	D	561	ASN
1	A	951	ASN
2	E	548	ASN
2	B	528	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	A1EF9	A	2303	-	39,39,39	0.48	1 (2%)	54,57,57	0.94	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1EF9	A	2303	-	-	1/31/50/50	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2303	A1EF9	C18-N09	2.13	1.52	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2303	A1EF9	C23-S01-N09	-3.69	100.78	107.36
4	A	2303	A1EF9	C34-N13-N12	2.68	106.78	104.36
4	A	2303	A1EF9	C32-C33-C34	2.67	106.31	103.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

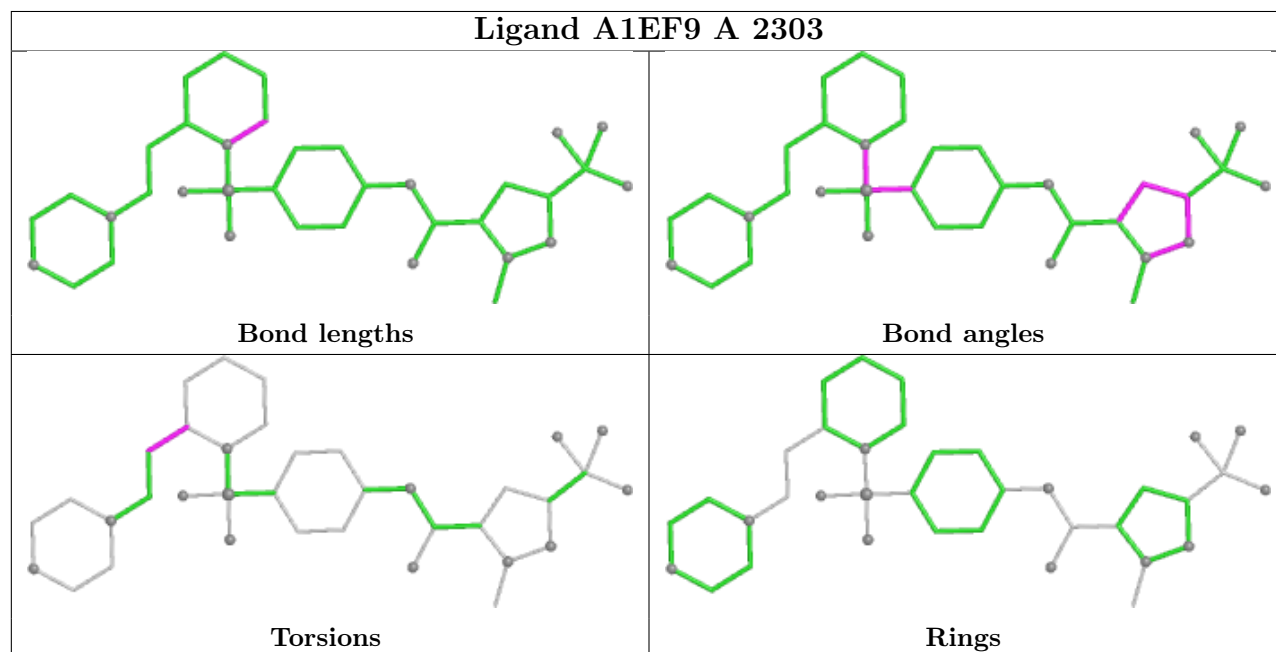
Mol	Chain	Res	Type	Atoms
4	A	2303	A1EF9	N09-C14-C16-C20

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.