



wwPDB EM Validation Summary Report ⓘ

May 5, 2026 – 06:15 PM JST

PDB ID : 21XO / pdb_000021xo
EMDB ID : EMD-68072
Title : Cryo-EM Structure of Nipah Virus Polymerase in complex with G671
Authors : Xue, L.; Gui, J.; Chang, T.; Pan, H.; Xiong, X.
Deposited on : 2026-01-03
Resolution : 2.92 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

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**
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

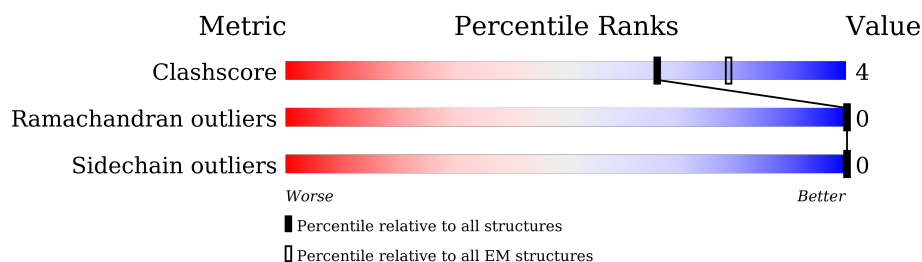
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





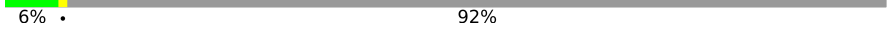
The reported resolution of this entry is 2.92 Å.

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 ≥ 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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13137 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.

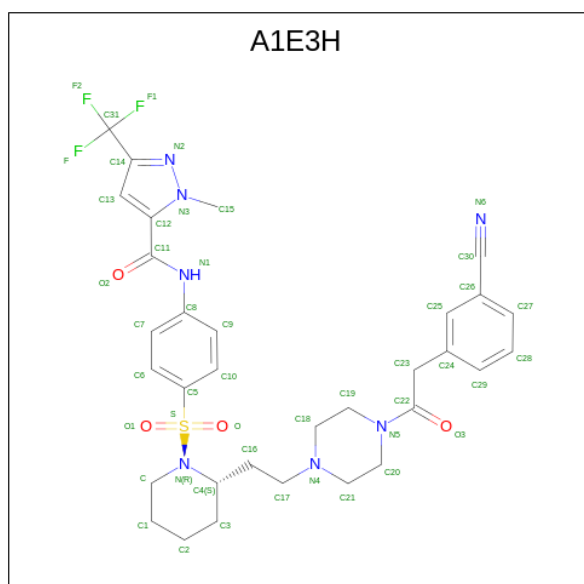
- Molecule 1 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1307	Total	C	N	O	S	0	0
			10518	6706	1796	1949	67		

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	148	Total	C	N	O	S	0	0
			1187	741	203	238	5		
2	C	52	Total	C	N	O	S	0	0
			412	260	71	77	4		
2	D	68	Total	C	N	O	S	0	0
			533	333	97	99	4		
2	E	56	Total	C	N	O	S	0	0
			438	276	77	81	4		

- Molecule 3 is {N}-[4-[(2 {S})-2-[2-[4-[2-(3-cyanophenyl)ethanoyl]piperazin-1-yl]ethyl]piperidin-1-yl]sulfonylphenyl]-2-methyl-5-(trifluoromethyl)pyrazole-3-carboxamide (CCD ID: A1E3H) (formula: C₃₂H₃₆F₃N₇O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	N	O	S	0
			47	32	3	7	4	1	

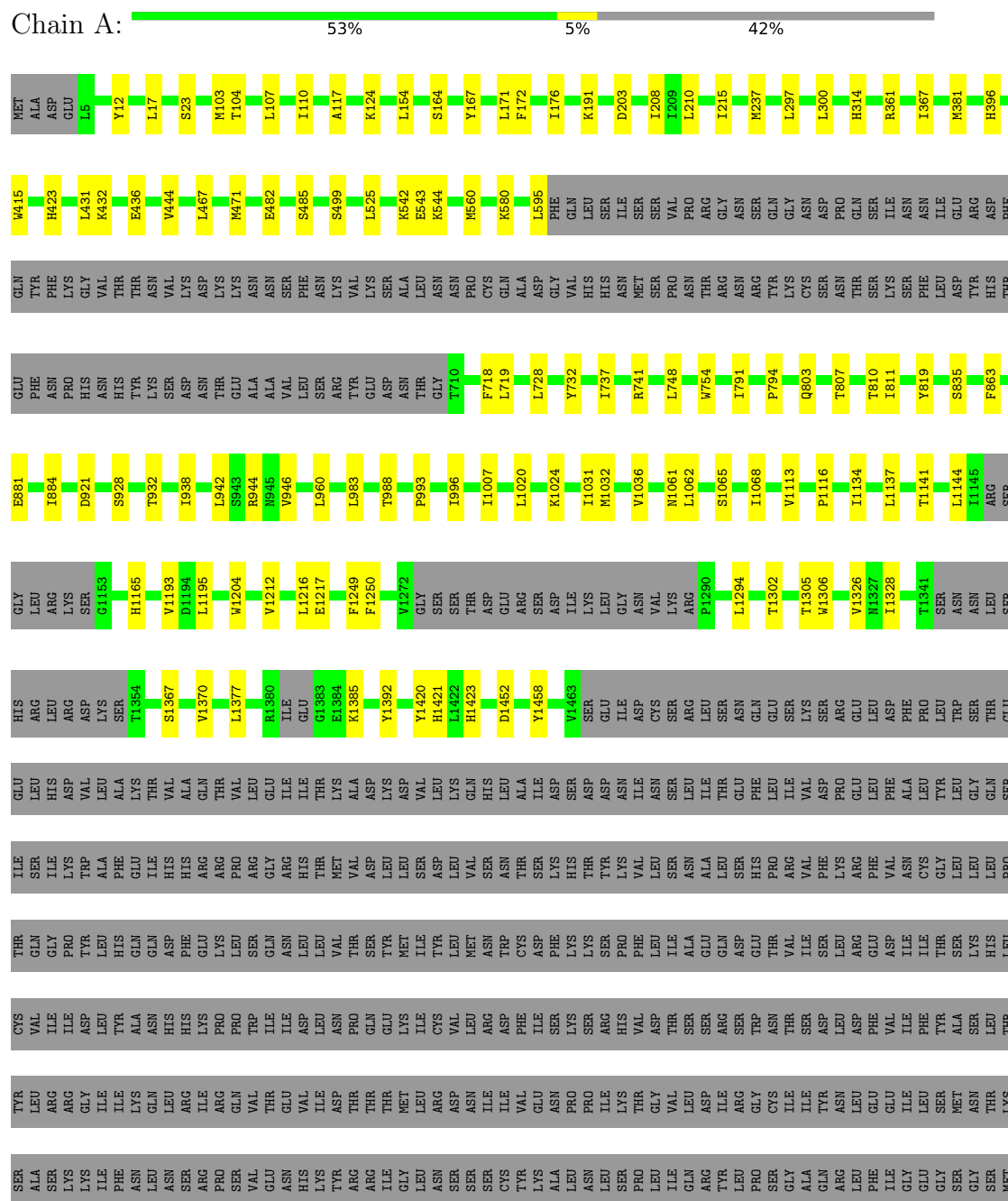
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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



[illegible]

- Molecule 2: Phosphoprotein

Chain B: 18% . 79%

J709	P544	SER	PRO	GLN	ASN	ASP	LEU	GLY	GLY	MET
	I547	ASP	GLY	PRO	LYS	ASP	SER	GLY	ASP	
	H548	PHE	SER	PRO	THR	THR	GLY	THR	CYS	LYS
	K549	SER	LYS	THR	THR	ASP	GLY	THR	GLY	GLU
	V556	THR	GLY	TRP	VAL	VAL	ASP	TRP	ASP	LEU
	L564	THR	ALA	SER	PRO	PRO	GLN	ASN	ASP	VAL
	P579	PHE	THR	ILE	GLY	GLY	LEU	PRO	PHE	ASN
	L584	PRO	HIS	ARG	GLY	ALA	PHE	THR	ASP	GLY
	P579	HIS	VAL	SER	PRO	LYS	VAL	VAL	SER	GLU
	GLY	ARG	ILE	LYS	ASP	ASP	PRO	PRO	ARG	ASN
	LYS	THR	SER	SER	LYS	GLU	GLU	PHE	ARG	ILE
	GLY	ASP	SER	PRO	SER	PHE	THR	ARG	ASN	ILE
	LYS	ARG	PRO	ASP	ALA	ALA	LEU	GLY	ASP	ILE
	GLU	LEU	PRO	LYS	VAL	GLY	TRP	ASP	PHE	GLY
	GLU	ASN	TYR	THR	LYS	SER	ASN	ASP	ASP	LEU
	ARG	TYR	GLN	GLU	GLU	SER	LEU	LEU	GLN	ILE
	LYS	HIS	GLY	ILE	GLU	SER	SER	TYR	SER	LYS
	GLY	ALA	GLY	VAL	PRO	GLU	ASP	ASP	THR	ASN
	LYS	ASN	LYS	GLY	GLN	ILE	VAL	PRO	THR	GLN
	ASN	LEU	VAL	ALA	LYS	VAL	GLY	LYS	ALA	GLY
PRO	GLY	ASN	GLN	ARG	GLY	ASP	ASP	ASN	ILE	
E593	ASP	TYR	ALA	GLN	LEU	ILE	GLY	THR	GLN	
I602	TYR	GLU	THR	THR	MET	PRO	PRO	GLY	LYS	
LEU	LEU	VAL	ASN	ALA	LEU	GLU	ILE	VAL	TYR	
GLU	GLU	GLN	ARG	ALA	CYS	ASP	ALA	CYS	GLY	
S610	THR	LEU	GLN	GLN	GLU	GLU	GLU	LEU	LYS	
PHE	THR	ASN	ARG	GLU	GLU	GLU	HIS	VAL	ARG	
ASN	ASN	ALA	ASN	GLU	PHE	TYR	TYR	VAL	SER	
VAL	GLU	SER	GLY	GLY	GLU	SER	TYR	ASP	ILE	
LYS	GLU	GLU	THR	THR	CYS	SER	GLY	ALA	ASN	
ASN	SER	ALA	PRO	MET	SER	VAL	LEU	LYS	GLN	
PHE	VAL	VAL	VAL	GLY	GLY	GLY	GLY	MET	PRO	
ARG	LEU	LYS	LYS	PRO	SER	GLY	VAL	ARG	ASP	
ASP	MET	GLY	GLU	GLU	GLU	LYS	VAL	ASP	PRO	
GLY	GLY	THR	THR	ASP	TYR	PRO	GLU	ALA	TRP	
SER	VAL	ASP	ARG	PRO	ASN	GLN	GLN	ASP	ALA	
ILE	LEU	LYS	LYS	ILE	PRO	ASN	ASN	GLY	GLN	
THR	ASN	SER	SER	ILE	ILE	SER	VAL	SER	THR	
ASN	GLU	GLU	GLU	ARG	ILE	GLY	GLY	GLU	LYS	
ASN	ILE	VAL	VAL	GLU	GLU	ILE	GLY	ASP	ASP	
ALA	W528	W528	ASP	THR	GLU	ARG	ARG	GLY	PHE	
ALA	W528	W528	ASP	ASN	ASN	ASN	ASN	GLY	ASP	
L533	W534	W534	ASN	ALA	SER	VAL	ASN	ASP	PRO	
Q632	Q632	Q632	ASP	LYS	LEU	GLN	VAL	VAL	GLN	
H536	H536	H536	SER	TYR	ILE	ILE	LEU	THR	VAL	
E537	E537	E537	LEU	PRO	ASN	ARG	ASP	THR	ASP	
Q539	Q539	Q539	ASP	SER	CYS	ASP	ASP	LEU	SER	
W540	W540	W540	ASP	ALA	GLN	ASN	ASN	VAL	GLY	
L681	L681	L681	LYS	GLY	GLN	LEU	LYS	VAL	TYR	
K541	K541	K541	TYR	THR	GLY	GLN	GLY	GLY	GLY	
W701	W701	W701	ILE	GLU	LYS	ALA	TYR	GLY	GLY	
E542	E542	E542	MET	ASN	ASP	LYS	THR	HIS	ASN	
W543	W543	W543	PRO	VAL	ALA	ASP	SER	GLY	GLY	

- Molecule 2: Phosphoprotein

ALA	GLY	ILE47	SER	PRO	GLN	ASN	ASP	LEU	GLY	GLY	ASP	LEU	GLY	GLY	MET
GLU	ALA	Y547	ASP	GLY	PRO	LYS	ASP	SER	GLY	GLY	GLU	SER	GLY	GLY	ASP
ASN	ALA	Y550	ASP	PRO	TYR	THR	THR	SER	GLU	GLU	GLU	THR	CYS	MET	LYS
ASP	GLN	Y550	SER	GLY	HIS	ASP	ASP	ASP	ALA	ASP	ASP	GLY	GLY	LYS	GLU
GLU	LEU	Y553	ASN	GLY	TRP	VAL	VAL	VAL	ASP	ASP	ASP	LEU	TRP	ASP	LEU
ILE	ARG	Y557	THR	ALA	SER	PRO	PRO	ILE	GLY	GLY	GLY	ASN	THR	ASP	VAL
GLN	GLU	Y557	PHE	THR	ILE	GLY	ALA	GLU	ALA	ALA	ALA	LEU	THR	ASP	ASN
GLU	ASP	Y560	PHE	ARG	GLU	ALA	ALA	GLU	ALA	ALA	ALA	LEU	THR	ASP	ASP
ILE	LEU	Y560	PRO	HIS	ARG	GLY	GLY	GLU	GLY	GLY	GLY	ALA	SER	VAL	GLY
ALA	ILE	Y579	HIS	VAL	SER	PRO	PRO	SER	PRO	GLU	GLU	VAL	GLY	GLU	LEU
ASN	LEU	Y579	ASP	ARG	ILE	LYS	LYS	ASP	ASP	PRO	PRO	VAL	PRO	ASP	ASN
THR	PRO	GLY	THR	GLY	SER	LYS	LYS	SER	GLU	GLU	GLU	PHE	ARG	ARG	ILE
VAL	GLU	LYS	ASP	SER	PRO	ASP	ASP	PRO	PHE	THR	THR	ARG	ASN	ASN	ILE
ASN	LEU	GLY	ARG	PRO	ASP	ALA	ALA	GLY	GLY	GLY	GLY	LEU	GLY	GLY	THR
ASP	ASN	LYS	LEU	PRO	LYS	VAL	VAL	THR	GLY	GLY	GLY	ASN	TRP	ASP	PHE
ILE	ILE	GLY	THR	PRO	THR	LYS	ASN	GLU	SER	SER	SER	LEU	ASP	ILE	GLN
ILE	GLU	GLU	TYR	GLN	GLU	GLU	VAL	VAL	GLY	GLY	GLY	LEU	ASP	LEU	THR
ASP	GLU	ARG	HIS	GLU	ILE	GLU	GLY	GLY	GLY	GLY	GLY	LEU	THR	THR	GLN
GLY	THR	LYS	ASP	GLY	VAL	PRO	ASP	VAL	GLY	GLY	GLY	ASN	THR	THR	ASN
ASN	ASN	GLY	LEU	THR	THR	GLY	GLN	ALA	GLN	GLY	GLY	LYS	GLY	GLY	GLN
ILE	SER	ASN	LEU	VAL	ALA	LYS	VAL	ARG	ALA	ASP	ASP	ALA	CYS	GLY	ARG
ASN	PHE	PRO	ASP	ASN	ARG	GLN	ASN	GLU	GLU	GLU	GLU	HIS	VAL	VAL	GLU
GLN	THR	GLU	GLY	GLY	THR	GLY	GLY	THR	GLY	GLY	GLY	GLY	THR	THR	GLY
ILE	ASP	VAL	GLY	GLY	GLY	GLY	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	GLY
ASN	ASN	VAL	GLY	GLY	GLY	GLY	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	GLY
ILE	GLN	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	GLY
GLN	THR	ILE	THR	GLN	GLN	GLN	VAL	GLN	GLU	GLU	GLU	GLU	GLY	GLY	GLN
ASN	ASN	ILE	THR	ASN	ARG	GLN	ASN	ARG	GLU	GLU	GLU	GLU	GLY	GLY	GLN
ILE	PHE	ILE	TYR	ALA	THR	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
GLU	VAL	GLY	TYR	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
ASP	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
ASN	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
ILE	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
GLN	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
ILE	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN
ASN	ASN	GLY	GLY	GLY											

Chain D: 8% . 90%

[illegible]

GLU
ILE
ALA
ASN
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	1638544	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: ZN, A1E3H

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	0.14	0/10735	0.36	0/14514
2	B	0.18	0/1196	0.47	0/1611
2	C	0.24	0/415	0.50	0/558
2	D	0.25	0/537	0.57	0/716
2	E	0.25	0/441	0.63	0/590
All	All	0.16	0/13324	0.39	0/17989

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	10518	0	10551	74	0
2	B	1187	0	1208	14	0
2	C	412	0	441	8	0
2	D	533	0	573	11	0
2	E	438	0	473	8	0
3	A	47	0	0	1	0
4	A	2	0	0	0	0
All	All	13137	0	13246	102	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 102 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:807:THR:O	1:A:810:THR:HG22	1.81	0.81
2:D:539:GLN:HG3	2:E:540:VAL:HB	1.70	0.73
1:A:17:LEU:HD22	1:A:237:MET:HB2	1.79	0.63
2:E:552:SER:HA	2:E:555:ARG:HE	1.66	0.60
2:C:560:THR:HG23	2:D:564:LEU:HD11	1.83	0.60

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	1295/2244 (58%)	1253 (97%)	42 (3%)	0	100	100
2	B	142/709 (20%)	140 (99%)	2 (1%)	0	100	100
2	C	50/709 (7%)	49 (98%)	1 (2%)	0	100	100
2	D	66/709 (9%)	66 (100%)	0	0	100	100
2	E	54/709 (8%)	53 (98%)	1 (2%)	0	100	100
All	All	1607/5080 (32%)	1561 (97%)	46 (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	1173/2046 (57%)	1173 (100%)	0	100	100
2	B	138/625 (22%)	138 (100%)	0	100	100
2	C	49/625 (8%)	49 (100%)	0	100	100
2	D	61/625 (10%)	61 (100%)	0	100	100
2	E	51/625 (8%)	51 (100%)	0	100	100
All	All	1472/4546 (32%)	1472 (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 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1264	HIS
2	B	605	GLN
2	C	539	GLN
2	B	686	ASN
2	C	534	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
3	A1E3H	A	3001	-	51,51,51	0.53	0	71,74,74	0.73	2 (2%)

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
3	A1E3H	A	3001	-	-	5/41/62/62	1/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	A1E3H	C12-C13-C14	2.37	106.01	103.64
3	A	3001	A1E3H	C14-N2-N3	2.35	106.48	104.36

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3001	A1E3H	O2-C11-N1-C8
3	A	3001	A1E3H	C12-C11-N1-C8
3	A	3001	A1E3H	C-N-S-O
3	A	3001	A1E3H	O3-C22-C23-C24
3	A	3001	A1E3H	C4-N-S-O

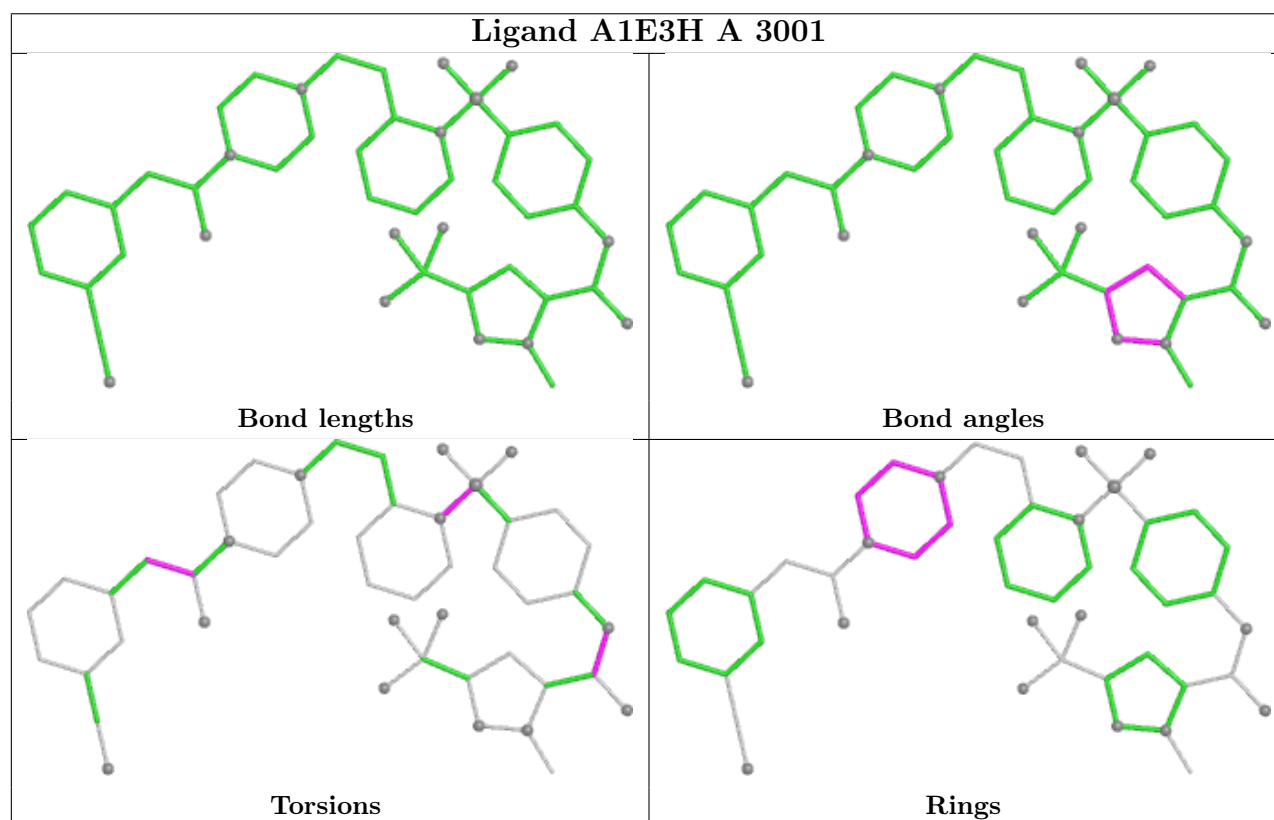
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3001	A1E3H	C18-C19-C20-C21-N4-N5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	A1E3H	1	0

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.