



Full wwPDB EM Validation Report ⓘ

Jun 28, 2026 – 12:48 AM 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 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**
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

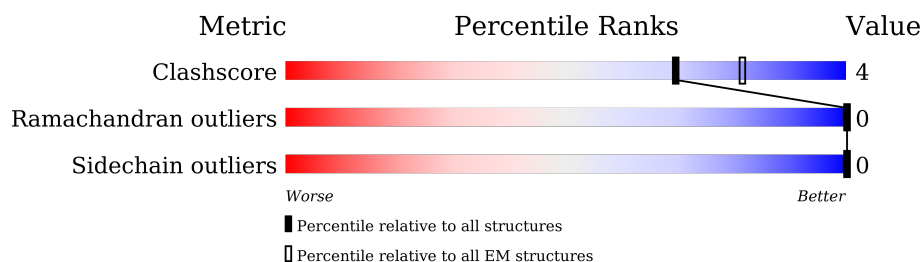
1 Overall quality at a glance

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 ≥ 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 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		

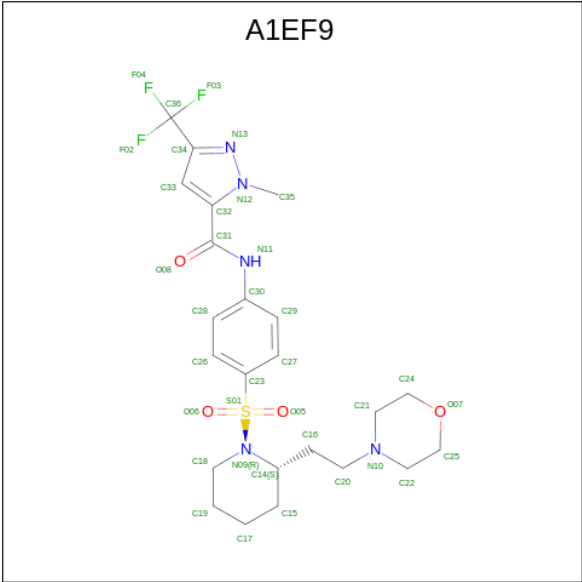
- Molecule 2 is a protein called Phosphoprotein.

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: C₂₃H₃₀F₃N₅O₄S) (labeled as "Ligand of Interest" by depositor).

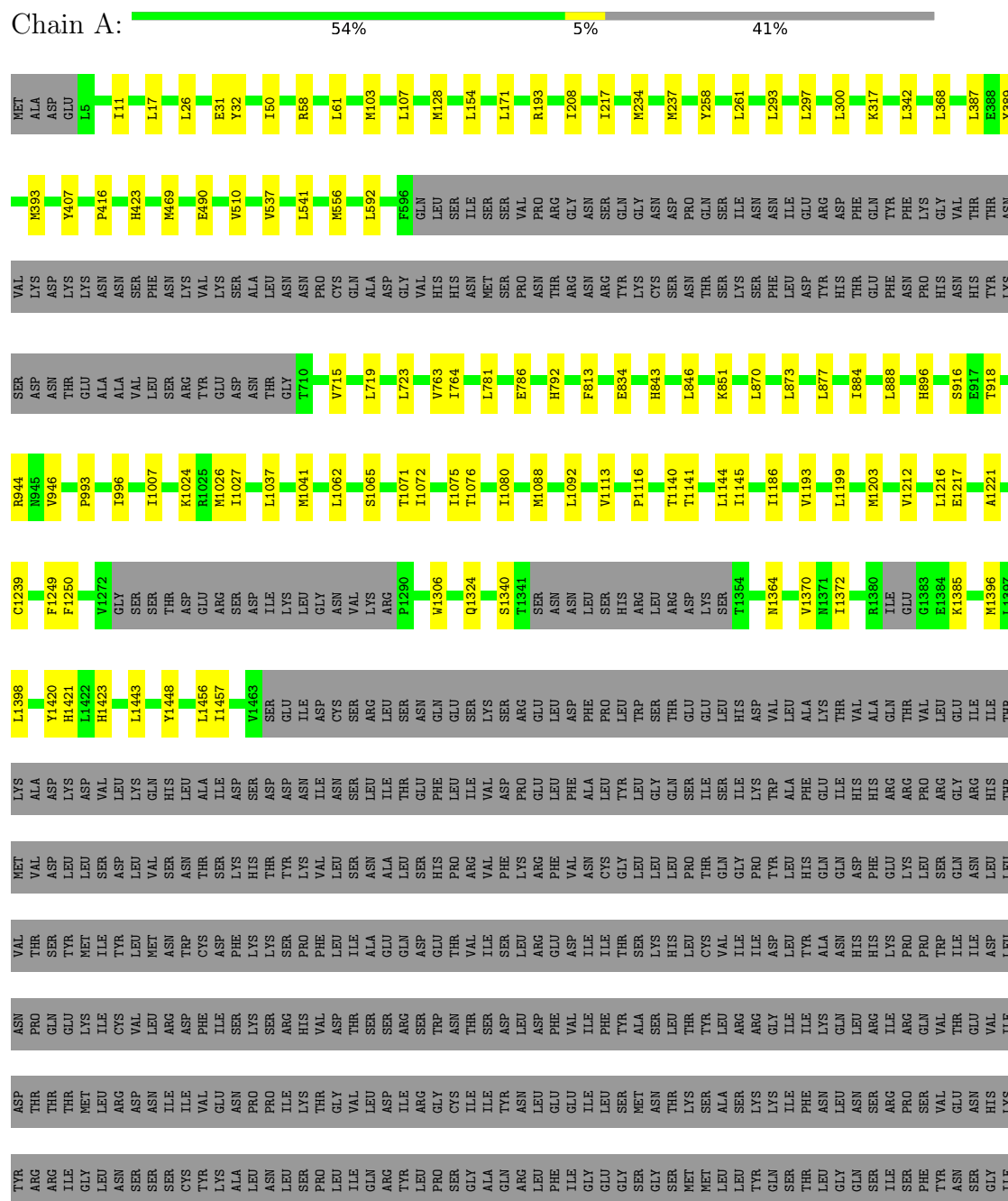


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	36	23	3	5	4	1	0

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



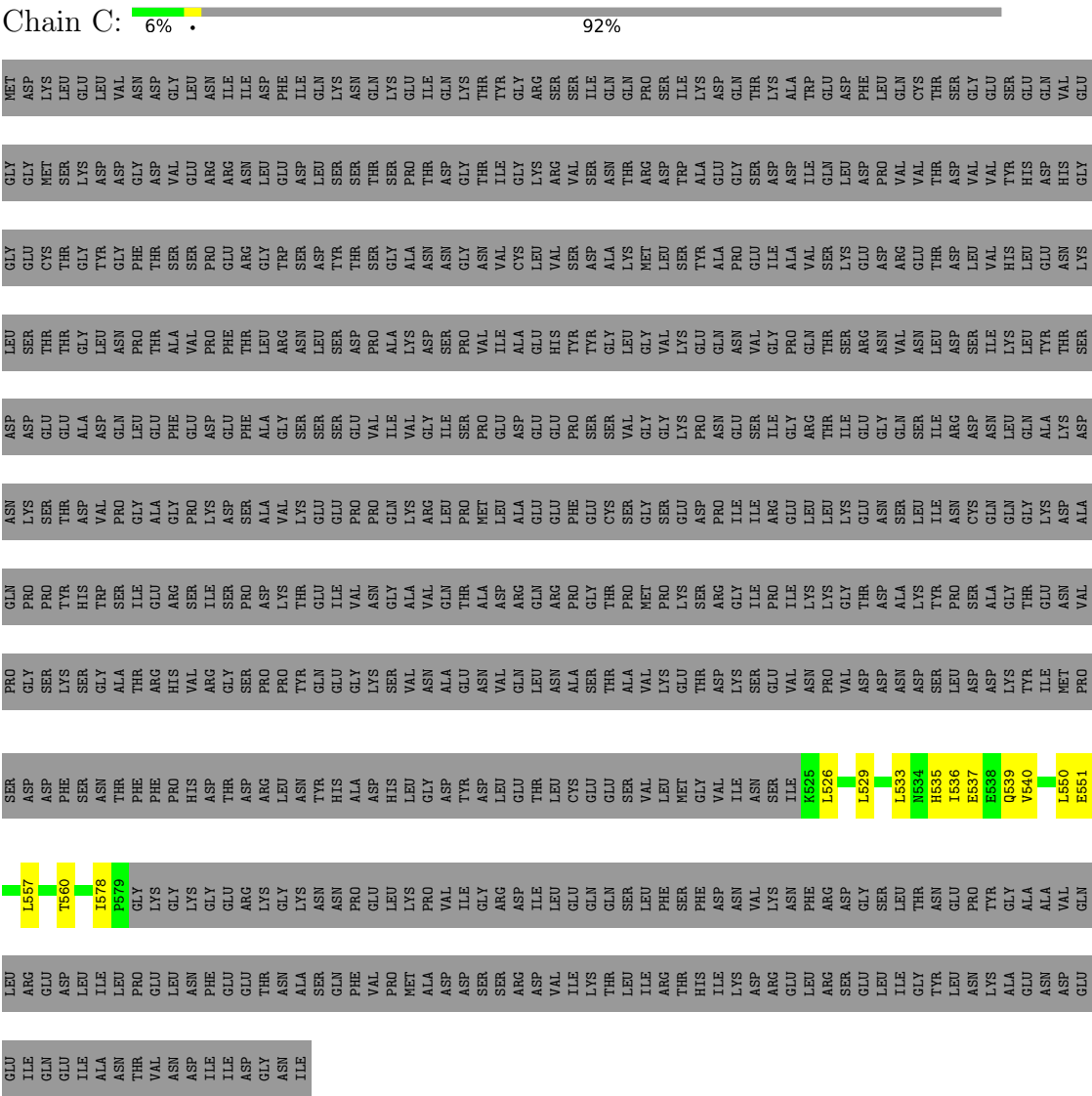
[illegible]

- Molecule 2: Phosphoprotein

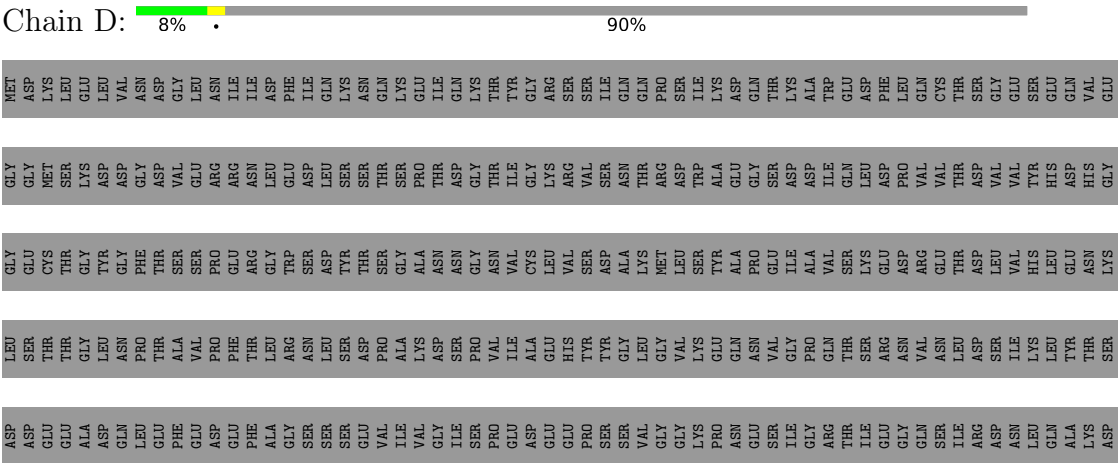
Chain B: 18% . 79%

1769	L564	SER	PRO	GLN	ASN	ASP	LEU	GLY	GLY	MET
		ASP	GLY	PRO	LYS	ASP	SER	SER	GLY	ASP
	M575	ASP	SER	PRO	ASN	GLY	THR	CYS	THR	LYS
	1576	PHE	LYS	THR	THR	GLY	GLY	THR	THR	SER
	P579	SER	SER	HIS	ASP	ALA	THR	GLY	THR	LYS
		ASN	GLY	TRP	VAL	ASP	LEU	TYR	ASP	LEU
	L594	THR	ALA	SER	PRO	GLN	ASN	GLY	ASP	VAL
		PHE	THR	ILE	PRO	GLY	PHE	THR	GLY	ASN
	L595	THR	ILE	GLY	GLY	THR	THR	THR	THR	ILE
		PHE	ARG	GLU	ALA	GLY	PHE	THR	GLY	GLY
	P596	PRO	HIS	ARG	GLY	GLY	ALA	LEU	ASP	GLY
		LYS	VAL	SER	PRO	LYS	VAL	SER	ASP	LEU
	L602	THR	GLY	SER	SER	LYS	ASP	PRO	ARG	ASN
		ARG	SER	PRO	PRO	GLY	GLU	PHE	GLU	ILE
	L594	ASP	PRO	ASP	ALA	ALA	LEU	ARG	GLY	GLY
	K595	LEU	VAL	ALA	LYS	VAL	LYS	ALA	PRO	GLY
	P596	GLY	ASN	GLN	ARG	GLY	ASP	ASN	THR	ILE
	L610	ASP	ALA	GLN	GLU	LEU	ILE	SER	ASP	GLN
		TYR	ASN	THR	THR	PRO	PRO	THR	GLY	LYS
	L610	LEU	VAL	ARG	ALA	ALA	ASP	GLY	GLY	GLY
PHE	GLU	GLN	ASP	GLU	GLU	GLU	LEU	LYS	ARG	
ASN	LEU	ASN	ARG	GLU	GLU	GLU	HIS	VAL	SER	
VAL	CYS	GLY	PRO	PHE	THR	PRO	TYR	VAL	ARG	
LYS	GLU	SER	GLY	GLY	GLY	SER	GLY	SER	ILE	
ASN	GLU	THR	THR	CYS	THR	GLY	ALA	ASN	GLN	
PHE	SER	ALA	PRO	SER	VAL	VAL	LEU	THR	GLN	
ARG	VAL	VAL	MET	GLY	GLY	GLY	GLY	ARG	PRO	
ASP	LEU	LYS	PRO	SER	GLY	GLY	VAL	ASP	SER	
GLY	MET	GLY	LYS	GLU	LYS	LYS	VAL	TRP	ILE	
SER	GLY	THR	SER	ASP	PRO	GLU	GLY	ALA	LYS	
LEU	VAL	VAL	ARG	PRO	ASN	GLN	GLY	ASP	GLN	
THR	ILE	LYS	SER	ILE	ILE	ASN	VAL	GLY	GLN	
ASN	ASN	SER	THR	ILE	GLY	ASN	THR	SER	THR	
GLU	GLU	GLY	VAL	ARG	GLY	VAL	GLY	ASP	LYS	
PRO	ILE	ILE	GLU	GLU	ILE	ILE	ILE	ASP	LYS	
K525	K525	THR	ASN	LYS	LEU	SER	GLN	ILE	TRP	
L533	L533	VAL	VAL	GLY	LYS	ILE	SER	LEU	ASP	
		ASP	ASP	THR	GLU	ARG	ARG	GLY	PHE	
E537	E537	ASP	ASP	ASN	GLY	ASN	ASN	GLY	ASP	
E538	E538	ASN	ASN	ALA	SER	ASN	VAL	GLN	PRO	
Q539	Q539	ASP	ASP	LYS	LEU	GLN	VAL	VAL	VAL	
V540	V540	SER	SER	THR	ILE	ILE	THR	SER	CYS	
K541	K541	LEU	LEU	PRO	ASN	ASP	ASP	THR	THR	
		ASP	ASP	SER	CYS	ASP	SER	LEU	ASN	
V548	V548	ASN	ASN	ALA	GLN	ASN	ILE	VAL	GLY	
P654	P654	LYS	LYS	GLY	GLN	ASN	ILE	GLY	THR	
L654	L654	TYR	THR	THR	GLY	GLN	LEU	VAL	SER	
		ILE	ILE	GLU	LYS	ALA	GLY	HIS	GLN	
E551	E551	MET	TYR	ASN	LYS	ALA	THR	ASP	ASN	
L667	L667	PRO	VAL	VAL	ALA	ASP	SER	GLY	GLN	
		ASN	ASN	ASN	ASN	ASP	THR	GLY	GLN	

- 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: ZN, A1EF9

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.

All (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
2:B:549:LYS:HD3	2:C:550:LEU:HB3	1.77	0.65
2:D:552:SER:HA	2:D:555:ARG:HE	1.61	0.65
2:C:526:LEU:HA	2:C:529:LEU:HD12	1.79	0.62
1:A:1062:LEU:HB2	1:A:1065:SER:HB3	1.82	0.62
2:C:537:GLU:HA	2:C:540:VAL:HG22	1.83	0.61
1:A:537:VAL:HG22	1:A:556:MET:HG2	1.85	0.57
2:B:564:LEU:HD11	2:E:560:THR:HG23	1.87	0.57
1:A:1041:MET:HG3	1:A:1186:ILE:HG21	1.87	0.56
1:A:1141:THR:H	1:A:1144:LEU:HD12	1.72	0.54
2:B:576:ILE:HD11	2:C:578:ILE:HD12	1.89	0.54
2:C:560:THR:HG23	2:D:564:LEU:HD11	1.89	0.53
2:B:602:ILE:HD11	2:E:579:PRO:HG2	1.91	0.52
1:A:1062:LEU:HD23	1:A:1203:MET:HE1	1.90	0.52
1:A:715:VAL:HG11	1:A:851:LYS:HB3	1.90	0.52
2:E:532:ARG:HA	2:E:535:HIS:CE1	2.45	0.52
1:A:1071:THR:HG23	1:A:1075:ILE:HD13	1.93	0.51
1:A:993:PRO:HD2	1:A:996:ILE:HD11	1.92	0.50
2:D:548:ASN:O	2:D:551:GLU:HG3	2.11	0.50
1:A:300:LEU:HD22	2:B:667:LEU:HD13	1.92	0.50
1:A:1076:THR:HG21	1:A:1140:THR:HG21	1.94	0.50
2:B:549:LYS:HE3	2:C:551:GLU:HG3	1.92	0.49
2:B:556:VAL:HG13	2:C:557:LEU:HD22	1.93	0.49
1:A:208:ILE:HG12	1:A:217:ILE:HG12	1.93	0.49
1:A:719:LEU:HG	1:A:884:ILE:HG12	1.94	0.49
1:A:1116:PRO:HG2	1:A:1216:LEU:HD11	1.94	0.49
2:D:537:GLU:HA	2:D:540:VAL:HG22	1.93	0.49
1:A:103:MET:HE1	1:A:208:ILE:HD12	1.93	0.49
2:D:532:ARG:HA	2:D:535:HIS:CE1	2.48	0.49
2:C:539:GLN:HG3	2:D:540:VAL:HB	1.95	0.49
2:B:647:THR:HG22	2:B:653:VAL:H	1.77	0.48
1:A:510:VAL:HG11	1:A:1080:ILE:HG22	1.95	0.48
1:A:368:LEU:HD13	1:A:541:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD22	1:A:342:LEU:HD21	1.96	0.48
2:B:539:GLN:HG3	2:C:540:VAL:HB	1.96	0.47
1:A:61:LEU:HD21	1:A:193:ARG:HH21	1.80	0.47
1:A:128:MET:HE1	1:A:1026:MET:HG2	1.97	0.47
1:A:944:ARG:HB3	1:A:1007:ILE:HD12	1.96	0.47
2:C:535:HIS:O	2:C:539:GLN:HG2	2.15	0.47
1:A:870:LEU:HD12	1:A:877:LEU:HD22	1.96	0.47
1:A:763:VAL:HB	1:A:781:LEU:HD13	1.97	0.46
2:B:537:GLU:HA	2:B:540:VAL:HG22	1.96	0.46
1:A:1221:ALA:HB1	1:A:1398:LEU:HD22	1.98	0.46
1:A:1421:HIS:HB3	1:A:1423:HIS:CD2	2.50	0.46
1:A:537:VAL:HG12	1:A:764:ILE:HG23	1.96	0.46
1:A:1088:MET:HE2	1:A:1456:LEU:HD11	1.96	0.46
2:B:654:PRO:HB3	2:B:664:ILE:HD11	1.98	0.46
1:A:888:LEU:HA	1:A:896:HIS:O	2.16	0.45
2:B:575:MET:HE3	2:B:594:LEU:HB3	1.99	0.45
1:A:317:LYS:HE2	1:A:317:LYS:HB3	1.85	0.45
1:A:786:GLU:HG3	1:A:792:HIS:HB2	1.99	0.45
1:A:1027:ILE:HD11	1:A:1037:LEU:HB2	1.98	0.45
1:A:237:MET:HB3	1:A:237:MET:HE3	1.86	0.45
2:B:533:LEU:O	2:B:537:GLU:HG2	2.17	0.44
1:A:32:TYR:CE1	1:A:50:ILE:HG12	2.52	0.44
1:A:723:LEU:HD11	1:A:834:GLU:HB2	1.99	0.43
2:B:595:LYS:HE3	2:E:573:SER:HB2	1.98	0.43
1:A:1193:VAL:HG13	1:A:1217:GLU:HB3	1.99	0.43
2:B:596:PRO:HB2	2:E:574:MET:SD	2.58	0.43
2:B:548:ASN:O	2:B:551:GLU:HG3	2.19	0.43
1:A:1372:ILE:HG21	1:A:1396:MET:HG3	2.01	0.43
1:A:1072:ILE:O	1:A:1076:THR:HB	2.18	0.43
1:A:407:TYR:HB3	1:A:416:PRO:HG3	2.00	0.42
1:A:592:LEU:HD23	1:A:1364:ASN:HD21	1.85	0.42
1:A:1250:PHE:O	1:A:1370:VAL:HA	2.20	0.42
1:A:1385:LYS:HE3	1:A:1385:LYS:HB3	1.87	0.42
1:A:389:TYR:CZ	1:A:393:MET:HG3	2.54	0.42
1:A:297:LEU:O	1:A:300:LEU:HB2	2.19	0.42
1:A:387:LEU:HB2	2:E:576:ILE:HB	2.01	0.42
2:B:538:GLU:HA	2:B:541:LYS:HE3	2.02	0.42
1:A:31:GLU:HB3	1:A:50:ILE:HG21	2.01	0.42
1:A:423:HIS:HB3	2:D:565:SER:HB3	2.00	0.42
1:A:1041:MET:HE1	1:A:1199:LEU:HB2	2.01	0.42
2:C:533:LEU:HA	2:C:536:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:PHE:CZ	1:A:873:LEU:HD13	2.54	0.41
2:D:564:LEU:HD23	2:D:564:LEU:HA	1.90	0.41
1:A:31:GLU:HB2	1:A:50:ILE:HD13	2.03	0.41
1:A:107:LEU:HG	1:A:171:LEU:HD22	2.02	0.41
1:A:154:LEU:HD21	1:A:946:VAL:HG22	2.03	0.41
1:A:1324:GLN:HG2	1:A:1448:TYR:CZ	2.55	0.41
2:E:537:GLU:HA	2:E:540:VAL:HG22	2.02	0.41
1:A:154:LEU:HD21	1:A:946:VAL:HA	2.03	0.41
1:A:469:MET:HE2	1:A:469:MET:HB3	1.93	0.41
1:A:1024:LYS:HB3	1:A:1024:LYS:HE2	1.80	0.41
1:A:1443:LEU:HD23	1:A:1443:LEU:HA	1.93	0.41
1:A:11:ILE:HG13	1:A:1145:ILE:HD11	2.02	0.41
2:D:550:LEU:O	2:D:553:ILE:HB	2.20	0.41
1:A:1306:TRP:CE2	1:A:1340:SER:HB3	2.55	0.41
1:A:17:LEU:HD22	1:A:237:MET:HB2	2.03	0.41
1:A:916:SER:O	1:A:918:THR:HG22	2.21	0.41
1:A:1092:LEU:HD22	1:A:1457:ILE:HD11	2.02	0.41
1:A:1113:VAL:HG13	1:A:1212:VAL:HG13	2.02	0.40
1:A:258:TYR:HD1	1:A:261:LEU:HD12	1.85	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1630/5080 (32%)	1579 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	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. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	213	ASN
1	A	313	HIS
1	A	365	HIS
1	A	380	HIS
1	A	519	ASN
1	A	753	ASN
1	A	770	ASN
1	A	951	ASN
1	A	1120	HIS
1	A	1264	HIS
2	B	528	ASN
2	B	648	ASN

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Mol	Chain	Res	Type
2	D	561	ASN
2	E	548	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.

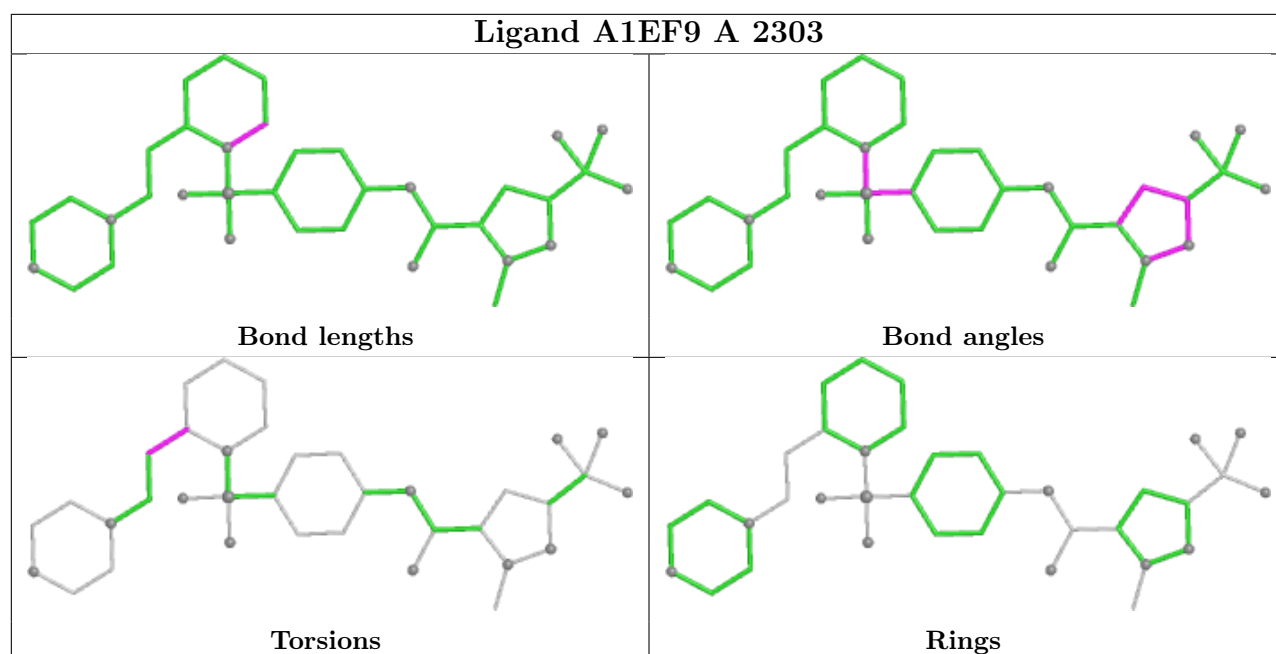
All (1) torsion outliers are listed below:

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.