



## Full wwPDB EM Validation Report ⓘ

May 5, 2026 – 06:12 PM JST

PDB ID : 9VXX / pdb\_00009vxx  
EMDB ID : EMD-65444  
Title : Cryo-EM Structure of Measles Virus Polymerase in complex with ERDRP-0519  
Authors : Xue, L.; Gui, J.; Chang, T.; Pan, H.; Xiong, X.  
Deposited on : 2025-07-20  
Resolution : 2.73 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](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

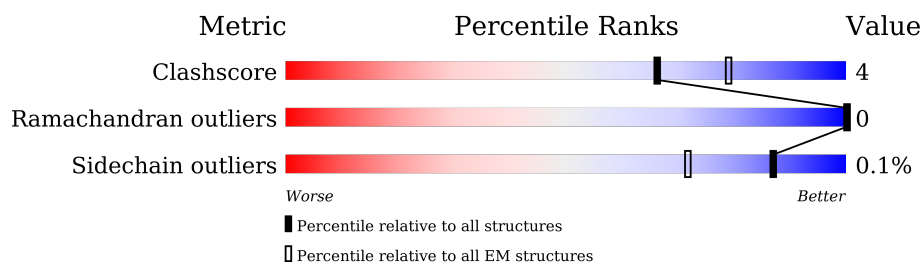
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.73 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	2183	
2	B	507	
2	C	507	
2	D	507	
2	E	507	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12608 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	1254	Total	C	N	O	S	0	0
			10077	6440	1742	1840	55		

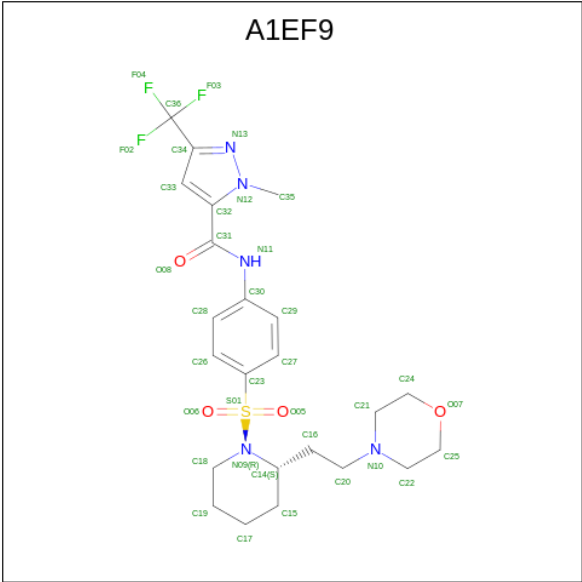
- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	148	Total	C	N	O	S	0	0
			1159	736	208	210	5		
2	C	47	Total	C	N	O	S	0	0
			372	233	65	73	1		
2	D	70	Total	C	N	O	S	0	0
			538	337	91	109	1		
2	E	55	Total	C	N	O	S	0	0
			425	269	74	81	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

- 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).

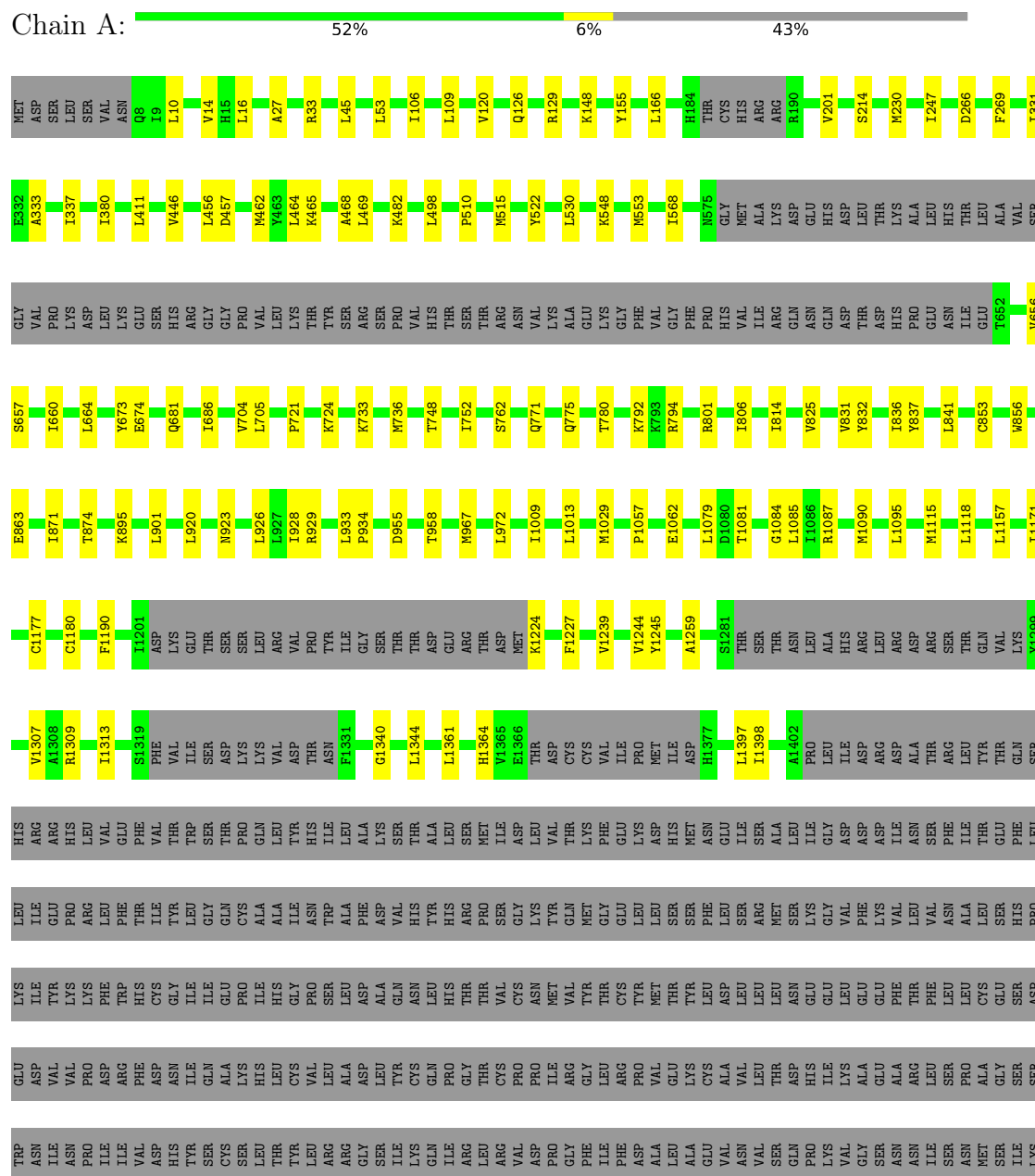


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	36	23	3	5	4	1	0

### 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



[illegible]

- Molecule 2: Phosphoprotein

Chain B:  25% 1% 71%

[illegible]

- Molecule 2: Phosphoprotein

Chain C:  8% 91%

[illegible]

PRO	LEU	GLU	THR	ASP	LYS	GLN	ASP	LYS
ASP	LYS	GLU	GLY	VAL	GLY	GLN	GLY	GLY
THR	PRO	GLY	ILE	THR	GLY	ALA	ILE	ILE
GLY	ILE	ASP	GLY	ASP	ASP	THR	ASP	GLN
ALA	ARG	TYR	THR	TYR	THR	LEU	GLU	ALA
SER	ARG	ASP	THR	ASP	ASP	LEU	GLY	ASP
ARG	SER	GLY	ASP	GLY	GLY	THR	ILE	THR
SER	GLY	GLU	GLY	GLY	LEU	ARG	THR	GLY
ILE	ARG	LEU	PHE	THR	ALA	ALA	HIS	VAL
ARG	ALA	SER	SER	THR	GLN	GLU	GLU	GLN
SER	LEU	ASP	VAL	CYS	ASP	LEU	LEU	SER
ILE	ALA	ASP	ASP	GLY	ASP	LEU	LEU	THR
ILE	ILE	VAL	ALA	ALA	VAL	GLY	THR	GLY
LYS	VAL	GLN	ARG	ARG	VAL	THR	THR	LEU
SER	LEU	ASP	LYS	LYS	ASP	THR	PRO	ASP
SER	LYS	ILE	SER	ASP	ASP	GLY	ILE	ARG
ARG	LYS	LYS	PRO	ARG	THR	PRO	ILE	SER
LEU	PRO	THR	THR	THR	THR	ASP	THR	THR
GLU	VAL	ALA	GLU	GLY	GLY	VAL	GLY	GLY
GLU	ALA	LEU	LEU	ALA	ALA	ASP	GLY	LEU
ASP	SER	ALA	SER	ALA	ALA	ASP	THR	GLY
ARG	GLN	LYS	PRO	GLY	LYS	ASP	PRO	GLY
LYS	GLN	1825	PRO	GLY	PRO	LYS	LYS	ASP
ARG	LEU	L336	GLY	GLY	LEU	GLY	LEU	ASP
TYR	GLN	L336	ALA	ALA	GLY	ALA	GLY	GLU
LEU	GLY	L339	PRO	PRO	LYS	THR	THR	SER
MET	MET	L349	ALA	ALA	GLY	GLY	LEU	GLU
THR	THR	L363	GLY	GLY	ASN	ASN	LEU	ASN
LEU	ASN	L367	VAL	VAL	VAL	VAL	ASN	SER
LEU	GLY	L370	CYS	CYS	VAL	PRO	GLY	ASP
ASP	ARG	M371	ASN	ASN	SER	ASN	GLY	GLY
ALA	GLY	ILE	ALA	ALA	VAL	SER	ALA	ALA
ASP	LEU	ALA	ALA	ALA	LEU	ARG	THR	ASP
LEU	LEU	ILE	LEU	ILE	LEU	ALA	ALA	GLU
ALA	LYS	PRO	ILE	ILE	PRO	SER	SER	GLY
LYS	GLU	GLY	GLN	GLN	GLY	THR	THR	TYR
PHE	PHE	LEU	GLN	GLN	THR	GLU	GLU	THR
HIS	GLN	LEU	LEU	LEU	LYS	THR	THR	ILE
GLN	LEU	LYS	LYS	LYS	ASP	THR	PRO	THR
MET	LYS	PRO	ASP	PRO	GLY	PRO	ILE	ASP
LEU	LEU	ASN	ASN	ASN	SER	ILE	LYS	ARG
MET	ILE	VAL	VAL	VAL	ASP	THR	ALA	GLY
ILE	GLY	ASP	GLY	GLY	ASP	GLY	LYS	THR
ILE	LYS	PRO	PRO	PRO	ASP	THR	THR	ALA
ILE	LYS	ALA	ALA	ALA	ASP	THR	THR	ALA
MET	VAL	ALA	ALA	ALA	ASP	SER	ASP	ALA
MET	SER	ASP	ASP	ASP	VAL	THR	ILE	THR
MET	SER	VAL	VAL	VAL	GLU	ARG	LYS	ARG
LYS	SER	ALA	ALA	ALA	GLY	GLY	GLY	THR

- Molecule 2: Phosphoprotein

Chain D:  12% . 86%

[illegible]

- Molecule 2: Phosphoprotein

Chain E:  8% . 89%

[illegible]





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2590005	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)	200	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	0.17	0/10302	0.34	0/13958
2	B	0.17	0/1168	0.36	0/1556
2	C	0.20	0/373	0.34	0/497
2	D	0.19	0/543	0.42	0/733
2	E	0.21	0/427	0.41	0/570
All	All	0.17	0/12813	0.35	0/17314

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	10077	0	10087	74	0
2	B	1159	0	1261	15	0
2	C	372	0	398	6	0
2	D	538	0	560	12	0
2	E	425	0	462	11	0
3	A	1	0	0	0	0
4	A	36	0	0	1	0
All	All	12608	0	12768	100	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 (100) 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:148:LYS:HD2	1:A:247:ILE:HA	1.70	0.74
1:A:1180:CYS:SG	1:A:1364:HIS:HE1	2.13	0.72
1:A:801:ARG:HD2	2:B:450:VAL:HG13	1.78	0.64
1:A:10:LEU:HD11	1:A:1087:ARG:HB3	1.79	0.63
1:A:456:LEU:HD13	1:A:510:PRO:HB2	1.80	0.62
1:A:933:LEU:HD12	1:A:934:PRO:HD2	1.81	0.62
1:A:530:LEU:HB3	1:A:705:LEU:HD22	1.82	0.61
1:A:568:ILE:HD11	1:A:686:ILE:HG21	1.83	0.60
1:A:853:CYS:HB2	1:A:874:THR:HG21	1.83	0.60
1:A:831:VAL:HG12	1:A:836:ILE:HG12	1.84	0.60
1:A:14:VAL:HG11	1:A:856:TRP:HB2	1.83	0.59
1:A:27:ALA:HB2	1:A:45:LEU:HD21	1.83	0.59
2:B:434:LEU:HD23	2:B:436:GLU:H	1.67	0.58
1:A:863:GLU:HG2	1:A:1009:ILE:HD12	1.85	0.58
1:A:1190:PHE:HB2	1:A:1361:LEU:HB3	1.85	0.58
1:A:871:ILE:HD13	1:A:895:LYS:HB3	1.88	0.55
1:A:1190:PHE:HE1	1:A:1313:ILE:HG23	1.72	0.55
1:A:126:GLN:HG2	1:A:129:ARG:HH12	1.71	0.54
1:A:721:PRO:HD2	1:A:724:LYS:HD2	1.87	0.54
1:A:411:LEU:HD11	1:A:446:VAL:HG13	1.89	0.53
1:A:120:VAL:HG11	1:A:928:ILE:HG21	1.90	0.53
1:A:1397:LEU:HD12	1:A:1398:ILE:HG13	1.89	0.53
1:A:664:LEU:HD21	4:A:2202:A1EF9:C33	2.39	0.53
1:A:1190:PHE:HE2	1:A:1340:GLY:HA3	1.75	0.52
1:A:515:MET:HE2	2:D:394:LEU:HD13	1.93	0.51
1:A:736:MET:HE1	2:E:375:PRO:HG2	1.92	0.51
1:A:522:TYR:HB2	1:A:553:MET:HE1	1.92	0.51
1:A:674:GLU:HB2	2:E:374:ILE:HD11	1.92	0.51
1:A:704:VAL:HG22	1:A:733:LYS:HG3	1.93	0.51
1:A:762:SER:HB3	1:A:806:ILE:HD12	1.93	0.50
1:A:794:ARG:HH22	2:B:506:MET:HG2	1.76	0.50
2:C:363:LEU:HD23	2:D:367:LEU:HD22	1.94	0.50
1:A:657:SER:HB2	1:A:780:THR:HG22	1.93	0.50
1:A:1090:MET:HG2	1:A:1095:LEU:HD12	1.93	0.49
1:A:681:GLN:HG2	2:D:372:ILE:HD13	1.95	0.49
2:B:364:GLU:HB2	2:E:363:LEU:HD11	1.95	0.49
1:A:748:THR:O	1:A:752:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:THR:HG22	1:A:1085:LEU:HD23	1.96	0.48
2:D:374:ILE:HB	2:D:377:LEU:HD22	1.94	0.48
2:D:325:ILE:HG22	2:D:328:ASP:H	1.79	0.48
1:A:1245:TYR:CD2	1:A:1259:ALA:HB2	2.49	0.48
2:E:342:LEU:HA	2:E:345:GLU:HG3	1.96	0.48
1:A:967:MET:HG2	1:A:972:LEU:HD23	1.94	0.47
2:B:339:LEU:HD21	2:C:339:LEU:HD13	1.97	0.47
1:A:457:ASP:HA	1:A:1029:MET:HE1	1.96	0.47
2:B:433:LEU:HD11	2:E:371:MET:HE1	1.96	0.47
1:A:656:VAL:HG21	1:A:792:LYS:HB3	1.96	0.46
2:C:349:ILE:HD12	2:D:353:ILE:HD12	1.97	0.46
1:A:920:LEU:HB2	1:A:1115:MET:HE2	1.96	0.46
2:C:370:ILE:HG22	2:D:377:LEU:HG	1.98	0.46
1:A:1084:GLY:HA2	1:A:1087:ARG:HE	1.81	0.46
2:C:367:LEU:HG	2:D:367:LEU:HD21	1.98	0.45
1:A:331:ILE:HG21	2:B:462:SER:HB3	1.97	0.45
1:A:929:ARG:HH12	1:A:1118:LEU:HB3	1.82	0.45
1:A:1062:GLU:HG2	1:A:1244:VAL:HG21	1.97	0.45
2:B:406:LEU:HA	2:B:409:VAL:HG12	1.99	0.45
1:A:1224:LYS:HE2	1:A:1239:VAL:HG21	1.98	0.45
2:C:336:LEU:HD12	2:C:339:LEU:HD12	1.99	0.44
2:E:346:VAL:HA	2:E:349:ILE:HD12	1.99	0.44
1:A:673:TYR:CD1	2:D:375:PRO:HG3	2.52	0.44
1:A:1307:VAL:HG11	1:A:1344:LEU:HB3	1.99	0.44
2:B:329:ASN:HA	2:B:332:ILE:HG12	1.99	0.44
1:A:530:LEU:HD22	1:A:705:LEU:HD13	1.98	0.44
2:B:374:ILE:HD11	2:B:395:LYS:HB2	1.99	0.44
2:B:352:GLN:HG2	2:B:355:ARG:HH22	1.82	0.44
1:A:464:LEU:HB3	1:A:1079:LEU:HD12	1.99	0.44
1:A:923:ASN:HD22	1:A:926:LEU:HD22	1.82	0.44
1:A:1190:PHE:CE2	1:A:1340:GLY:HA3	2.52	0.44
1:A:462:MET:HA	1:A:465:LYS:HE3	2.00	0.43
1:A:201:VAL:HG12	1:A:214:SER:HA	2.00	0.43
1:A:1057:PRO:HG2	1:A:1157:LEU:HD11	2.00	0.43
1:A:1171:ILE:HD11	1:A:1177:CYS:HB2	1.99	0.43
2:E:328:ASP:O	2:E:332:ILE:HG12	2.19	0.43
1:A:1013:LEU:HD11	1:A:1095:LEU:HD13	1.99	0.43
2:B:336:LEU:HG	2:E:335:LYS:HE3	2.01	0.43
2:D:353:ILE:HA	2:D:356:GLN:HG2	2.00	0.43
1:A:832:TYR:HE1	1:A:837:TYR:HB2	1.84	0.42
1:A:955:ASP:HB3	1:A:958:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:HH21	1:A:53:LEU:HD22	1.83	0.42
1:A:109:LEU:HD22	1:A:901:LEU:HB3	2.01	0.42
1:A:266:ASP:HA	1:A:269:PHE:HD2	1.84	0.42
1:A:660:ILE:HG23	1:A:825:VAL:HG22	2.01	0.42
1:A:1224:LYS:HB3	1:A:1227:PHE:HB3	2.01	0.42
2:D:379:LYS:HD2	2:D:379:LYS:HA	1.86	0.42
1:A:16:LEU:HD22	1:A:230:MET:HB2	2.01	0.42
1:A:468:ALA:HB3	1:A:548:LYS:HE2	2.02	0.42
2:B:336:LEU:HG	2:E:335:LYS:HG2	2.02	0.42
1:A:333:ALA:O	1:A:337:ILE:HG13	2.20	0.41
2:B:367:LEU:HD12	2:E:363:LEU:HD22	2.01	0.41
1:A:841:LEU:HD23	1:A:1309:ARG:HH12	1.84	0.41
1:A:664:LEU:HD23	1:A:664:LEU:HA	1.92	0.41
1:A:380:ILE:HG23	1:A:814:ILE:HA	2.03	0.41
1:A:148:LYS:HD3	1:A:155:TYR:CE2	2.55	0.41
2:B:346:VAL:O	2:B:350:LYS:HG3	2.20	0.41
2:E:331:LYS:O	2:E:335:LYS:HG3	2.21	0.41
1:A:469:LEU:HD21	1:A:498:LEU:HD13	2.02	0.40
1:A:771:GLN:HG3	1:A:832:TYR:HB2	2.02	0.40
1:A:106:ILE:HG23	1:A:166:LEU:HD22	2.04	0.40
1:A:482:LYS:HE3	1:A:482:LYS:HB2	1.92	0.40
2:D:374:ILE:HA	2:D:375:PRO:HD3	1.97	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	1240/2183 (57%)	1209 (98%)	31 (2%)	0	100	100
2	B	142/507 (28%)	139 (98%)	3 (2%)	0	100	100
2	C	45/507 (9%)	45 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	68/507 (13%)	66 (97%)	2 (3%)	0	100	100
2	E	53/507 (10%)	52 (98%)	1 (2%)	0	100	100
All	All	1548/4211 (37%)	1511 (98%)	37 (2%)	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	1113/1945 (57%)	1112 (100%)	1 (0%)	88	94
2	B	132/416 (32%)	132 (100%)	0	100	100
2	C	45/416 (11%)	45 (100%)	0	100	100
2	D	64/416 (15%)	64 (100%)	0	100	100
2	E	50/416 (12%)	50 (100%)	0	100	100
All	All	1404/3609 (39%)	1403 (100%)	1 (0%)	87	94

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

Mol	Chain	Res	Type
1	A	775	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	55	ASN
1	A	358	HIS
1	A	404	HIS
1	A	697	HIS
1	A	775	GLN
1	A	923	ASN

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Mol	Chain	Res	Type
1	A	924	ASN
1	A	1066	HIS
1	A	1124	ASN
1	A	1265	GLN
1	A	1334	GLN
2	C	329	ASN

### 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, 1 is 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	2202	-	39,39,39	0.66	0	54,57,57	1.16	4 (7%)

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	2202	-	-	4/31/50/50	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2202	A1EF9	C23-S01-N09	-5.40	97.74	107.36
4	A	2202	A1EF9	O05-S01-N09	3.36	113.10	106.97
4	A	2202	A1EF9	C34-N13-N12	2.70	106.80	104.36
4	A	2202	A1EF9	C32-C33-C34	2.59	106.23	103.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2202	A1EF9	O08-C31-N11-C30
4	A	2202	A1EF9	C32-C31-N11-C30
4	A	2202	A1EF9	C14-N09-S01-O06
4	A	2202	A1EF9	C14-N09-S01-O05

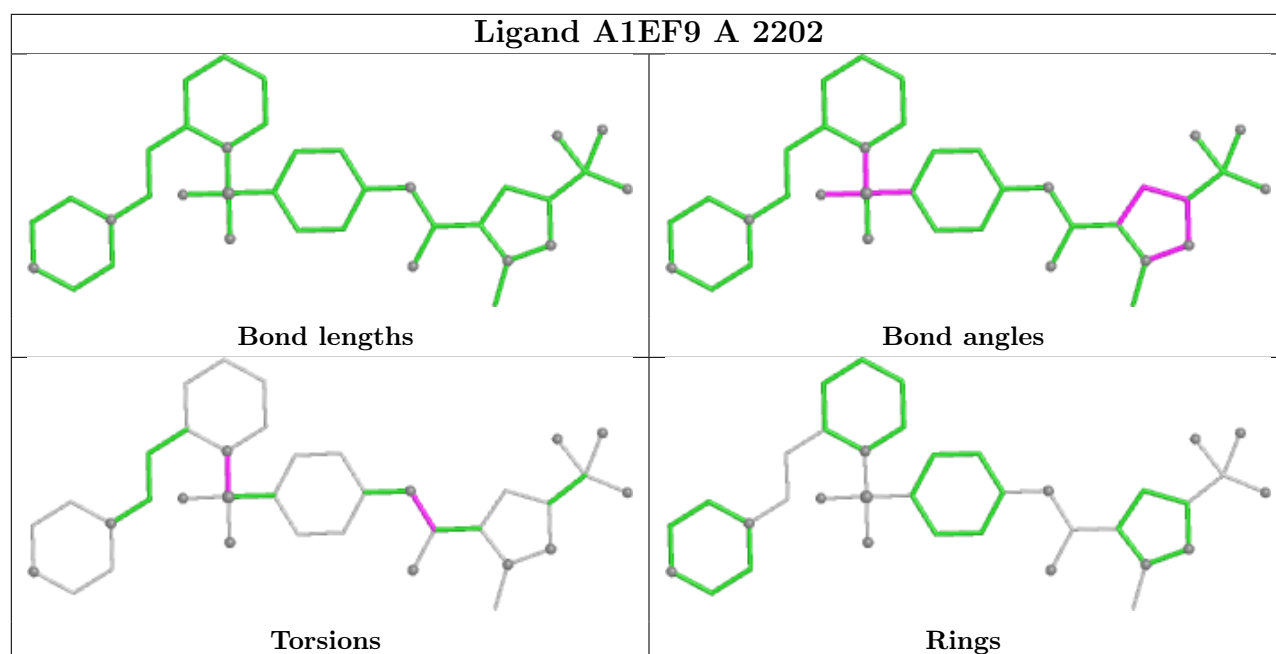
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2202	A1EF9	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.