



wwPDB EM Validation Summary 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 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

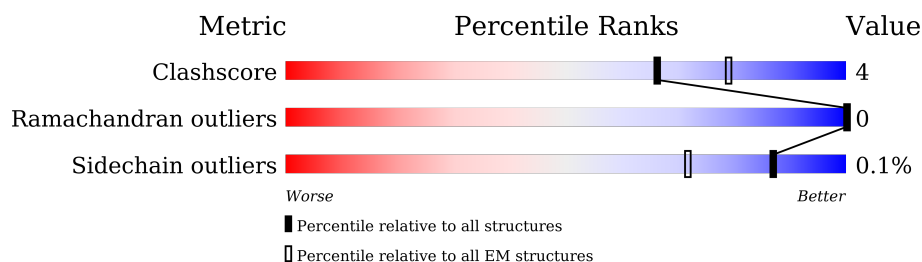
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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 ≥ 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		

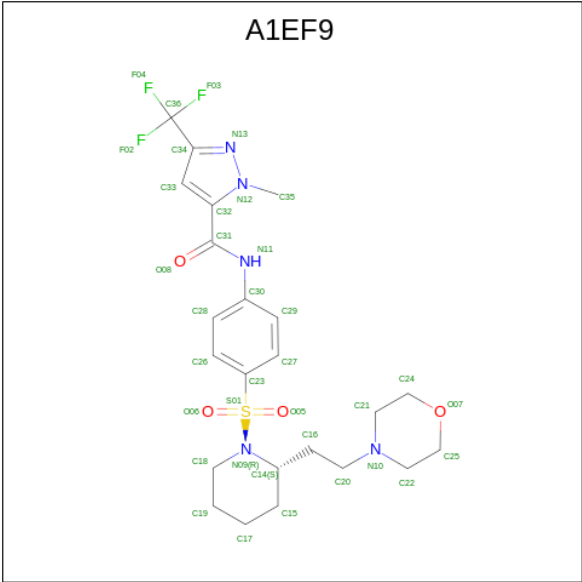
- Molecule 2 is a protein called Phosphoprotein.

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

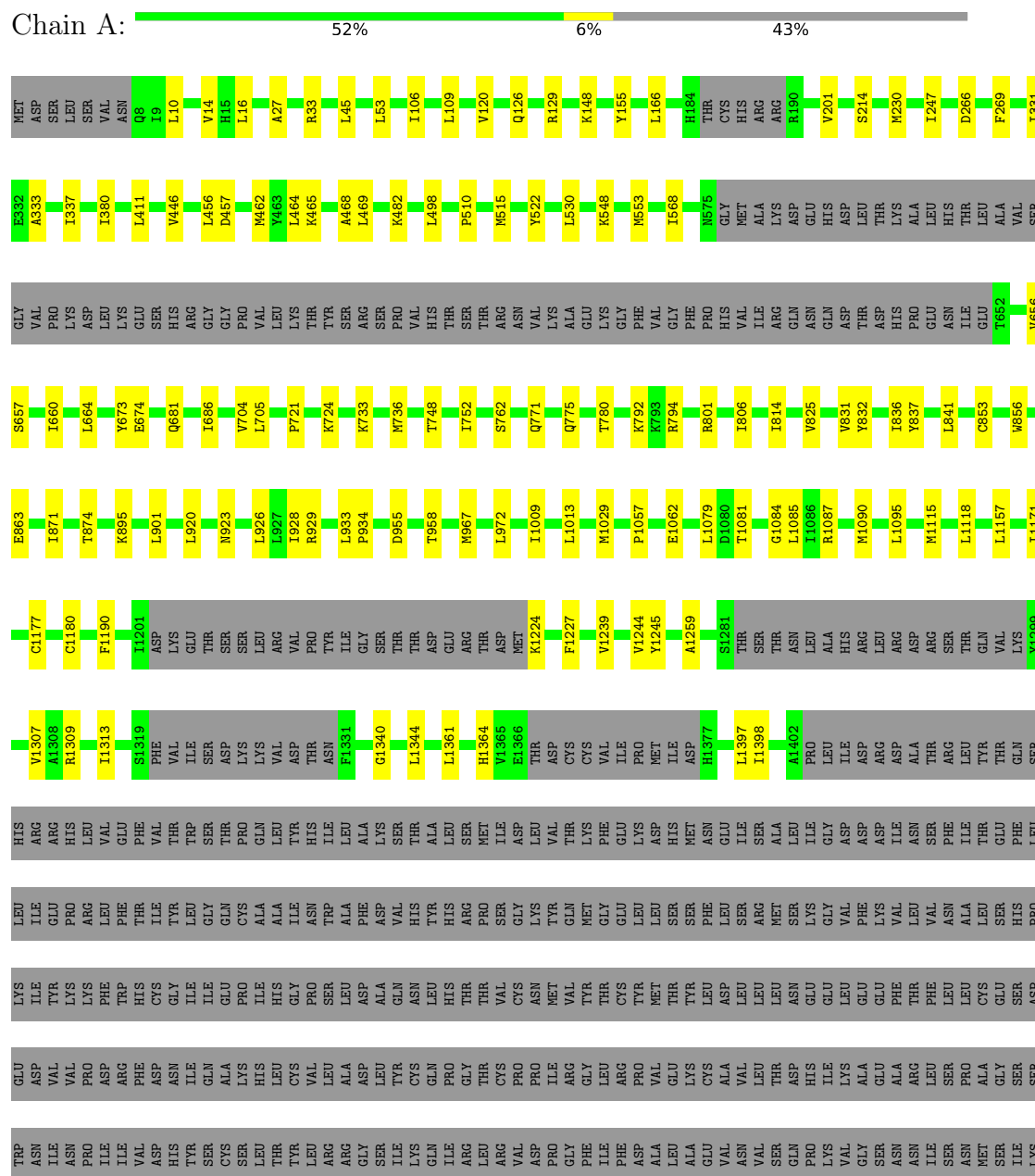


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	36	23	3	5	4	1	0

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:  25% 1% 71%

VAL	GLU	THR	ASP	LYS	SER	MET
GLU	GLU	GLU	VAL	GLY	LYS	ALA
LEU	GLY	ILE	GLU	ILE	PRO	GLY
ASN	GLY	ALA	THR	GLN	CYS	GLN
PRO	ASP	SER	ALA	ASP	LEU	GLN
ASP	THR	LEU	GLU	ALA	SER	ALA
L384	ASP	LEU	GLY	ASP	ARG	ARG
K395	THR	THR	GLY	SER	ILE	HIS
L406	ASP	GLY	ILE	ILE	GLY	VAL
V409	LEU	ALA	HIS	VAL	THR	ASN
L410	PHE	THR	GLU	GLN	GLY	GLY
K411	SER	GLN	LEU	SER	GLY	LEU
GLY	ASP	CYS	LEU	GLY	GLY	GLU
PRO	VAL	ALA	LYS	LEU	ALA	CYS
VAL	GLN	ARG	LEU	ASP	PRO	ILE
VAL	ASP	LYS	GLN	GLY	ARG	ARG
ALA	ILE	SER	SER	ASP	ILE	ALA
SER	LYS	PRO	ARG	SER	ARG	LEU
ARG	THR	SER	GLY	THR	GLY	LYS
GLN	ALA	GLU	ASN	LEU	GLN	ALA
LEU	LEU	PRO	ASN	SER	GLY	ALA
GLN	ALA	SER	PHE	GLY	SER	PRO
GLY	LYS	GLY	PRO	GLY	ILE	ILE
MET	I325	PRO	LYS	ASP	GLY	GLY
THR	N329	GLY	LEU	ASP	SER	SER
ASN	ALA	ALA	GLY	GLU	ASP	LEU
GLY	I332	PRO	LYS	SER	ASP	ALA
ARG	ALA	GLY	THR	GLU	ASP	VAL
THR	L336	GLY	LEU	ASN	ALA	GLU
SER	L339	VAL	VAL	SER	GLU	GLU
S429	L433	PRO	VAL	ASP	THR	ALA
L433	L434	GLU	PRO	VAL	LEU	MET
L435	V246	CYS	PRO	ASP	GLY	ALA
E436	K350	VAL	PRO	ILE	ILE	TRP
V450	K351	SER	ASN	GLY	PRO	SER
THR	K352	ASN	ALA	THR	GLU	ILE
S462	R355	ALA	ARG	LEU	SER	ASP
M506	E364	LEU	ALA	THR	GLN	ASN
K507	L367	ILE	SER	GLY	ALA	PRO
	I374	GLU	THR	TYR	SER	GLY
	P375	SER	THR	ALA	SER	GLY
	GLY	GLY	ILE	ILE	THR	ASP
	LEU	GLY	LYS	ARG	GLN	ARG
	LYS	THR	THR	GLY	CYS	THR
	ASP	ILE	ASP	ILE	THR	GLU
	PRO	SER	ALA	SER	ASP	GLU
	ASN	PRO	ARG	LEU	ASP	GLU
	PRO	ARG	LEU	MET	HIS	ALA
	THR	SER	ALA	GLY	VAL	ALA
	PRO	ASP	ALA	THR	GLY	GLY
	THR	SER	ALA	PHE	GLY	SER
	ASN	GLN	SER	ARG	GLY	SER
	ALA	ASN	PHE	ALA	ALA	GLY
	SER	ASN	CYS	SER	VAL	THR

- Molecule 2: Phosphoprotein

Chain C: 8% 91%

[illegible]

Chain E: 8% 89%





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.

The worst 5 of 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

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
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 [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	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. 5 of 13 such sidechains are listed below:

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

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 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:

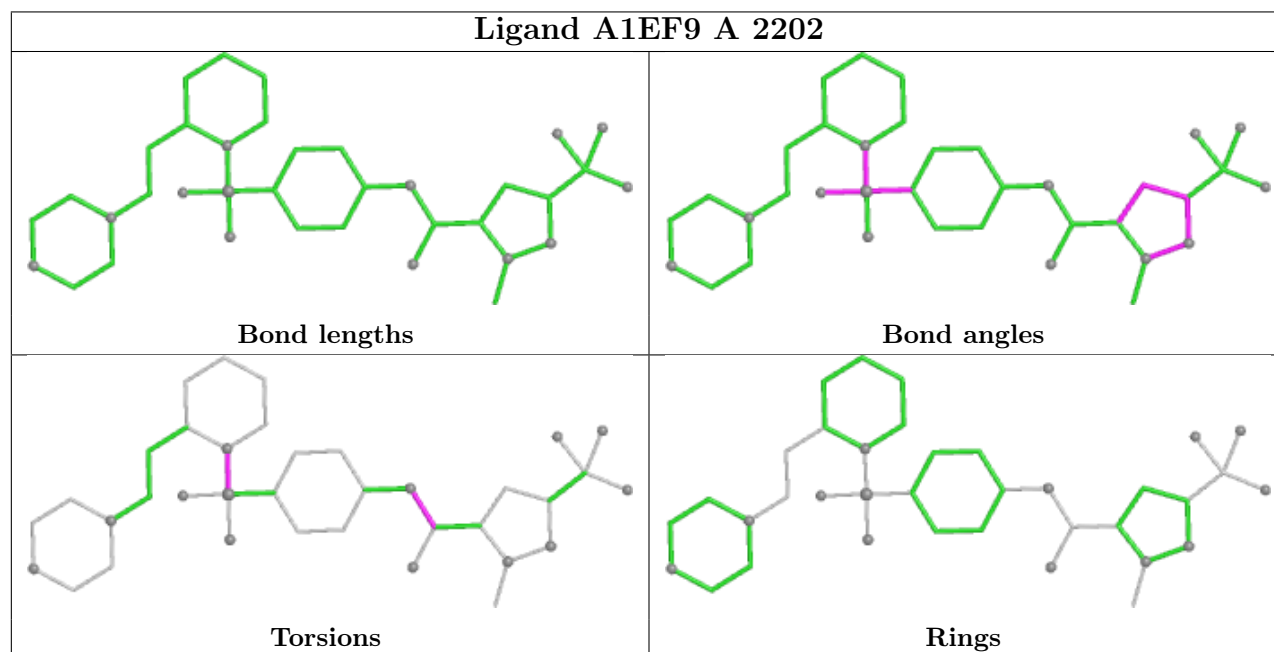
Mol	Chain	Res	Type	Atoms
4	A	2202	A1EF9	O08-C31-N11-C30
4	A	2202	A1EF9	C32-C31-N11-C30
4	A	2202	A1EF9	C14-N09-S01-O06
4	A	2202	A1EF9	C14-N09-S01-O05

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.