



## Full wwPDB EM Validation Report ⓘ

Sep 14, 2025 – 12:19 AM JST

PDB ID : 9KNZ / pdb\_00009knz  
EMDB ID : EMD-62467  
Title : ERDRP-0519-bound Nipah virus L-P complex  
Authors : Wang, Y.R.; Zhang, H.Q.  
Deposited on : 2024-11-19  
Resolution : 3.00 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 Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

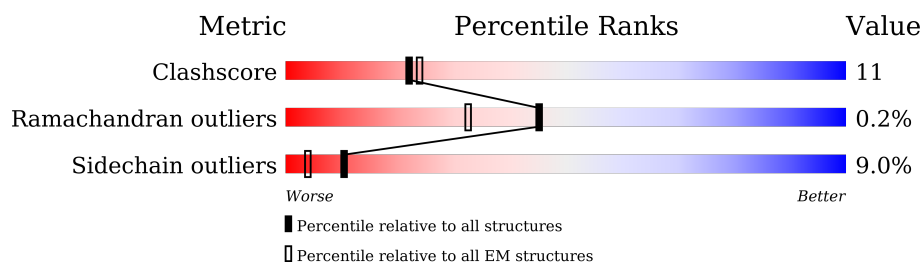
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12436 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.

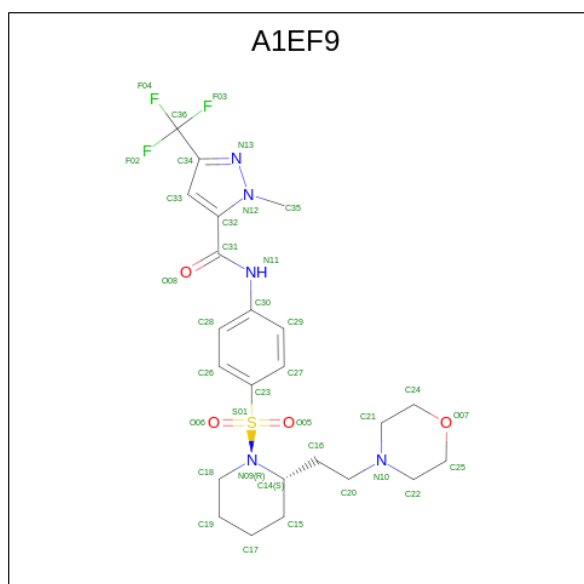
- Molecule 1 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1272	Total	C	N	O	S	0	0
			10233	6514	1754	1899	66		

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	51	Total	C	N	O	S	0	0
			400	252	70	77	1		
2	C	53	Total	C	N	O	S	0	0
			418	264	74	79	1		
2	D	117	Total	C	N	O	S	0	0
			922	573	161	183	5		
2	E	54	Total	C	N	O	S	0	0
			425	269	75	80	1		

- Molecule 3 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).



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





[illegible]







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162836	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)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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	0.18	1/10442 (0.0%)	0.42	2/14115 (0.0%)
2	B	0.19	0/401	0.66	1/539 (0.2%)
2	C	0.18	0/420	0.47	0/565
2	D	0.19	0/926	0.51	0/1245
2	E	0.22	0/427	0.61	0/575
All	All	0.18	1/12616 (0.0%)	0.45	3/17039 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1175	LYS	C-O	-5.28	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1179	ASN	CB-CA-C	-5.74	97.91	109.68
1	A	486	VAL	N-CA-C	-5.25	107.64	112.83
2	B	520	VAL	N-CA-C	-5.15	106.43	111.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ASN	Peptide
2	B	536	ILE	Peptide

## 5.2 Too-close contacts

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	10233	0	10273	192	0
2	B	400	0	433	24	0
2	C	418	0	451	20	0
2	D	922	0	959	40	0
2	E	425	0	460	26	0
3	A	36	0	0	0	0
4	A	2	0	0	0	0
All	All	12436	0	12576	282	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 11.

All (282) 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)
2:B:557:LEU:O	2:B:561:ASN:HB2	1.72	0.88
1:A:1042:ASN:HD22	1:A:1181:ARG:HB3	1.41	0.85
1:A:1176:LEU:HD23	1:A:1176:LEU:O	1.81	0.79
2:B:532:ARG:HG3	2:C:533:LEU:HB2	1.66	0.77
1:A:463:LEU:HD13	1:A:517:PRO:HB2	1.69	0.73
2:B:543:ILE:HG13	2:B:544:PRO:HD3	1.70	0.73
2:B:551:GLU:O	2:B:555:ARG:HB3	1.91	0.70
1:A:15:CYS:SG	1:A:181:ARG:NH1	2.65	0.70
1:A:481:ASP:OD1	1:A:481:ASP:N	2.14	0.69
1:A:921:ASP:OD2	1:A:968:ASN:ND2	2.25	0.69
2:D:546:ILE:HD13	2:E:547:ILE:HG21	1.72	0.69
1:A:924:ARG:NH2	1:A:998:GLY:O	2.26	0.69
1:A:147:ASN:O	1:A:149:HIS:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ASP:O	1:A:446:ASN:ND2	2.27	0.67
1:A:919:LEU:HB3	1:A:922:GLU:HG3	1.76	0.66
2:B:556:VAL:O	2:B:560:THR:OG1	2.13	0.66
1:A:852:LYS:HZ2	1:A:886:THR:HG1	1.42	0.66
2:B:533:LEU:HB3	2:E:532:ARG:NH1	2.11	0.65
1:A:1107:PHE:O	1:A:1111:ARG:NH1	2.30	0.64
2:C:543:ILE:HG13	2:C:544:PRO:HD3	1.79	0.63
1:A:1180:ARG:HG3	1:A:1180:ARG:HH11	1.64	0.63
2:C:532:ARG:O	2:C:536:ILE:HG13	1.97	0.63
1:A:439:THR:OG1	1:A:442:ASP:OD1	2.17	0.63
1:A:543:GLU:HG2	1:A:544:LYS:HG2	1.81	0.63
1:A:972:THR:OG1	1:A:974:ASP:OD1	2.17	0.63
2:B:522:ASN:HB2	2:B:525:LYS:HE3	1.81	0.63
1:A:1200:ARG:HG2	1:A:1204:TRP:CD1	2.34	0.63
2:D:544:PRO:HA	2:D:547:ILE:HB	1.81	0.63
1:A:1181:ARG:O	1:A:1182:GLN:NE2	2.32	0.62
1:A:385:LYS:NZ	1:A:874:GLY:O	2.32	0.62
1:A:1188:SER:OG	1:A:1189:ASN:OD1	2.16	0.62
1:A:1436:VAL:HG13	1:A:1438:GLN:H	1.65	0.62
1:A:141:ARG:HG2	1:A:142:ARG:H	1.65	0.62
1:A:1378:ASP:H	1:A:1380:ARG:HG3	1.65	0.62
2:E:525:LYS:HD2	2:E:526:LEU:HD12	1.81	0.61
1:A:525:LEU:HD11	1:A:748:LEU:HD12	1.83	0.61
1:A:1368:ARG:NH2	1:A:1369:TYR:OH	2.29	0.60
2:B:551:GLU:O	2:B:555:ARG:CB	2.49	0.60
1:A:1227:GLY:O	1:A:1228:ARG:NH2	2.34	0.60
1:A:1112:ARG:HH22	1:A:1437:GLY:HA3	1.68	0.59
1:A:136:LEU:HD23	1:A:137:ILE:HG22	1.86	0.58
1:A:1243:ASN:ND2	1:A:1425:LYS:O	2.28	0.58
2:D:682:ILE:O	2:D:686:ASN:ND2	2.36	0.58
2:E:528:ASN:O	2:E:532:ARG:HG3	2.02	0.58
1:A:138:THR:HG21	1:A:1229:TYR:HD2	1.68	0.58
1:A:361:ARG:HH22	1:A:544:LYS:HZ3	1.50	0.58
1:A:1374:ASN:HB3	1:A:1396:MET:HE2	1.86	0.58
1:A:1126:SER:OG	1:A:1127:LEU:N	2.37	0.58
2:C:544:PRO:HA	2:C:547:ILE:HG13	1.85	0.58
1:A:255:ASP:OD1	1:A:256:ILE:N	2.34	0.57
1:A:561:ARG:NH1	1:A:564:GLN:OE1	2.35	0.57
1:A:1311:ASN:ND2	1:A:1314:CYS:SG	2.78	0.57
2:B:532:ARG:HA	2:B:535:HIS:NE2	2.20	0.57
1:A:1364:ASN:N	1:A:1364:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:PRO:HA	2:B:547:ILE:HG22	1.87	0.56
2:D:673:LYS:O	2:D:678:ARG:NH2	2.38	0.56
2:C:534:ASN:OD1	2:C:534:ASN:N	2.35	0.56
2:D:532:ARG:NH2	2:E:537:GLU:OE1	2.38	0.55
1:A:302:ASP:OD1	1:A:303:GLU:N	2.39	0.55
1:A:480:LYS:HA	1:A:536:ASN:HD22	1.72	0.55
1:A:1046:GLY:O	1:A:1061:ASN:ND2	2.38	0.55
1:A:231:THR:OG1	1:A:234:MET:SD	2.63	0.55
1:A:963:THR:HG23	1:A:964:GLU:HG3	1.89	0.55
1:A:1328:ILE:HB	1:A:1453:ASN:HB2	1.89	0.55
2:B:544:PRO:O	2:B:548:ASN:HB3	2.07	0.54
1:A:250:THR:O	1:A:254:SER:OG	2.25	0.54
1:A:1200:ARG:HG2	1:A:1204:TRP:HD1	1.71	0.54
2:D:675:ARG:HE	2:D:678:ARG:HE	1.54	0.54
1:A:1067:SER:O	1:A:1071:THR:HG23	2.07	0.54
1:A:1154:LEU:HG	1:A:1155:GLN:OE1	2.07	0.54
1:A:561:ARG:O	1:A:565:VAL:HG23	2.07	0.54
1:A:1191:CYS:SG	1:A:1193:VAL:HG22	2.48	0.54
1:A:1387:ASP:N	1:A:1387:ASP:OD1	2.41	0.54
2:E:532:ARG:O	2:E:535:HIS:ND1	2.38	0.54
2:E:535:HIS:CD2	2:E:539:GLN:HE22	2.27	0.53
2:D:534:ASN:O	2:D:537:GLU:HG3	2.09	0.53
2:D:538:GLU:HA	2:D:541:LYS:HD3	1.90	0.53
2:E:541:LYS:O	2:E:545:LYS:NZ	2.42	0.53
1:A:132:ILE:HD11	1:A:1004:LEU:HD13	1.91	0.53
1:A:489:ARG:O	1:A:489:ARG:NH1	2.38	0.53
1:A:907:LYS:HG2	1:A:911:ARG:HH21	1.74	0.53
1:A:1378:ASP:HB2	1:A:1380:ARG:HE	1.74	0.52
1:A:999:PHE:HE1	1:A:1173:LEU:HD22	1.75	0.52
1:A:919:LEU:O	1:A:921:ASP:N	2.43	0.52
1:A:788:ASP:OD1	1:A:788:ASP:N	2.36	0.52
1:A:1180:ARG:HG3	1:A:1180:ARG:NH1	2.25	0.51
1:A:466:ASP:OD1	1:A:467:LEU:N	2.44	0.51
1:A:832:ASP:OD1	1:A:832:ASP:N	2.41	0.51
1:A:247:MET:O	1:A:251:THR:HG22	2.10	0.51
1:A:1328:ILE:HG13	1:A:1329:ASP:OD1	2.09	0.51
1:A:375:GLU:OE2	1:A:378:ARG:NH1	2.43	0.51
1:A:164:SER:OG	1:A:249:GLU:OE2	2.28	0.51
1:A:351:HIS:HD2	1:A:1257:LEU:HD11	1.76	0.51
1:A:1067:SER:HG	1:A:1069:THR:HG1	1.58	0.51
2:D:674:ASP:HB2	2:D:677:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:550:LEU:HD23	2:C:553:ILE:HD11	1.92	0.50
2:D:658:ASP:HA	2:D:661:ARG:HD2	1.93	0.50
1:A:1120:HIS:C	1:A:1122:ILE:H	2.18	0.50
1:A:1377:LEU:HD11	1:A:1381:ILE:HG23	1.93	0.50
1:A:1214:TYR:OH	1:A:1434:ALA:O	2.20	0.50
1:A:958:GLN:O	1:A:958:GLN:NE2	2.44	0.50
2:D:559:LYS:HA	2:D:562:THR:HG22	1.94	0.50
1:A:513:GLU:HB3	1:A:1085:PRO:HB2	1.93	0.50
1:A:722:ASP:OD1	1:A:723:LEU:N	2.45	0.50
1:A:536:ASN:OD1	1:A:537:VAL:N	2.45	0.50
2:D:550:LEU:O	2:D:553:ILE:HG12	2.12	0.50
1:A:1176:LEU:HD23	1:A:1176:LEU:C	2.37	0.49
1:A:144:GLU:HB3	1:A:146:ILE:HG23	1.94	0.49
1:A:1186:ILE:HD13	1:A:1188:SER:HB3	1.95	0.49
2:C:546:ILE:O	2:C:549:LYS:HG3	2.11	0.49
1:A:131:ASN:HD22	1:A:1029:HIS:HE1	1.58	0.49
1:A:1141:THR:OG1	1:A:1142:LYS:N	2.46	0.49
2:E:568:GLU:HB3	2:E:570:HIS:ND1	2.27	0.49
2:B:535:HIS:ND1	2:B:536:ILE:HG13	2.27	0.49
2:D:553:ILE:O	2:D:556:VAL:HG12	2.12	0.49
2:C:543:ILE:O	2:C:546:ILE:HG13	2.13	0.49
1:A:131:ASN:HD22	1:A:1029:HIS:CE1	2.31	0.49
1:A:1325:ARG:O	1:A:1328:ILE:HG12	2.13	0.49
1:A:713:ASP:OD1	1:A:714:THR:N	2.41	0.48
1:A:1298:ILE:O	1:A:1302:THR:OG1	2.22	0.48
2:C:544:PRO:HA	2:C:547:ILE:CG1	2.43	0.48
1:A:304:ALA:HB3	1:A:307:LEU:HD12	1.94	0.48
1:A:887:HIS:ND1	1:A:898:ASP:OD2	2.41	0.48
1:A:776:ASP:OD1	1:A:776:ASP:N	2.46	0.48
1:A:1373:SER:OG	1:A:1375:ASP:OD1	2.31	0.48
1:A:440:ILE:HA	1:A:443:CYS:SG	2.54	0.48
1:A:542:LYS:HD2	1:A:551:ARG:HB3	1.95	0.48
2:E:559:LYS:HD3	2:E:559:LYS:HA	1.59	0.48
1:A:283:ILE:O	1:A:287:VAL:HG23	2.13	0.48
1:A:522:GLU:O	1:A:526:SER:OG	2.21	0.48
1:A:65:ARG:NH2	1:A:187:SER:OG	2.47	0.47
1:A:1328:ILE:HG22	1:A:1453:ASN:N	2.29	0.47
1:A:1014:ASP:OD2	1:A:1017:THR:OG1	2.29	0.47
1:A:961:ILE:HG23	1:A:965:PHE:HB3	1.96	0.47
1:A:499:SER:OG	1:A:500:THR:N	2.48	0.47
1:A:914:PHE:CE2	1:A:961:ILE:HD12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:SER:OG	1:A:1189:ASN:N	2.47	0.47
2:D:567:ILE:HG23	2:D:570:HIS:HB3	1.96	0.47
1:A:351:HIS:CD2	1:A:1257:LEU:HD11	2.50	0.47
1:A:1091:GLY:O	1:A:1451:VAL:HG11	2.15	0.47
2:D:668:ILE:O	2:D:672:ILE:HG22	2.15	0.47
1:A:275:LEU:HD11	1:A:337:PHE:CE2	2.50	0.46
1:A:811:ILE:N	1:A:812:PRO:HD2	2.30	0.46
2:B:535:HIS:HA	2:B:538:GLU:OE2	2.15	0.46
1:A:245:ARG:HH21	1:A:269:TRP:CD1	2.34	0.46
2:D:527:ILE:O	2:D:531:MET:HG2	2.16	0.46
1:A:1086:ASN:OD1	1:A:1088:MET:N	2.49	0.46
1:A:1237:GLN:H	1:A:1237:GLN:CD	2.23	0.46
1:A:1221:ALA:O	1:A:1225:MET:HG3	2.15	0.46
1:A:408:ARG:HG2	1:A:413:GLY:HA2	1.98	0.46
2:E:550:LEU:O	2:E:553:ILE:HG13	2.17	0.46
1:A:542:LYS:HB3	1:A:542:LYS:HE3	1.64	0.45
1:A:1237:GLN:O	1:A:1238:ILE:HD13	2.15	0.45
1:A:1243:ASN:OD1	1:A:1425:LYS:HB3	2.16	0.45
1:A:1298:ILE:HG13	1:A:1299:ARG:N	2.30	0.45
2:B:533:LEU:HB3	2:E:532:ARG:HH12	1.80	0.45
1:A:361:ARG:HH12	1:A:544:LYS:HZ2	1.64	0.45
1:A:18:ASP:OD1	1:A:18:ASP:N	2.49	0.45
1:A:1292:LYS:HG2	1:A:1294:LEU:H	1.82	0.45
2:B:526:LEU:HD11	2:E:525:LYS:HG3	1.99	0.45
2:C:532:ARG:HH22	2:D:534:ASN:HD22	1.64	0.45
1:A:717:ALA:HB2	1:A:855:CYS:SG	2.57	0.45
1:A:757:LYS:O	1:A:761:ARG:NE	2.50	0.45
1:A:1150:ARG:HD3	1:A:1150:ARG:HA	1.84	0.45
1:A:924:ARG:HH11	1:A:1169:GLN:HE21	1.64	0.45
1:A:1083:ASN:N	1:A:1083:ASN:OD1	2.50	0.45
2:D:675:ARG:NE	2:D:678:ARG:HE	2.15	0.45
1:A:48:GLU:OE1	1:A:51:ARG:NH1	2.50	0.45
1:A:975:VAL:HG21	1:A:1167:TYR:CE1	2.51	0.45
1:A:529:TYR:HD1	1:A:529:TYR:H	1.65	0.45
2:C:568:GLU:OE2	2:E:572:VAL:HG23	2.16	0.45
1:A:59:LYS:HE2	1:A:59:LYS:HB2	1.76	0.45
1:A:246:MET:O	1:A:250:THR:OG1	2.32	0.45
1:A:1380:ARG:HB3	1:A:1385:LYS:HD3	1.99	0.45
2:C:541:LYS:O	2:C:544:PRO:HD2	2.18	0.44
1:A:39:GLN:HE21	1:A:88:TYR:H	1.65	0.44
1:A:922:GLU:HB3	1:A:925:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:PRO:HD2	1:A:1157:LYS:NZ	2.33	0.44
1:A:1377:LEU:HD13	1:A:1380:ARG:H	1.82	0.44
2:B:539:GLN:NE2	2:C:540:VAL:HG23	2.33	0.44
1:A:378:ARG:NH2	1:A:786:GLU:O	2.49	0.44
1:A:975:VAL:HG21	1:A:1167:TYR:HE1	1.82	0.44
2:C:536:ILE:HA	2:C:539:GLN:HB2	1.98	0.44
2:D:679:SER:HA	2:D:682:ILE:HG22	1.99	0.44
2:D:682:ILE:HG13	2:D:686:ASN:HD21	1.83	0.44
1:A:900:ALA:HB2	1:A:1368:ARG:NH1	2.33	0.44
2:E:532:ARG:C	2:E:535:HIS:HD1	2.24	0.44
2:B:524:ILE:HD12	2:B:525:LYS:N	2.33	0.44
2:D:521:ILE:HG13	2:D:522:ASN:N	2.32	0.44
2:E:549:LYS:HB3	2:E:549:LYS:HE3	1.77	0.44
1:A:945:ASN:OD1	1:A:945:ASN:N	2.48	0.43
1:A:1384:GLU:H	1:A:1384:GLU:HG3	1.67	0.43
2:B:549:LYS:HA	2:B:549:LYS:HD3	1.81	0.43
1:A:140:ASP:HB3	1:A:145:ILE:HG23	2.00	0.43
1:A:1163:SER:OG	1:A:1164:HIS:ND1	2.50	0.43
2:B:529:LEU:HD11	2:C:529:LEU:HD21	2.01	0.43
2:B:557:LEU:HB3	2:E:557:LEU:HD22	1.99	0.43
2:D:538:GLU:O	2:D:542:GLU:HG3	2.18	0.43
1:A:357:PHE:HE2	1:A:895:ILE:HD11	1.83	0.43
1:A:754:TRP:CD1	1:A:754:TRP:H	2.35	0.43
2:E:553:ILE:HA	2:E:556:VAL:HG12	2.00	0.43
1:A:423:HIS:CG	2:B:555:ARG:HB2	2.53	0.43
1:A:1445:ILE:H	1:A:1445:ILE:HG13	1.48	0.43
1:A:573:SER:O	1:A:577:LYS:NZ	2.43	0.43
1:A:361:ARG:HH12	1:A:544:LYS:NZ	2.17	0.43
1:A:1311:ASN:ND2	1:A:1314:CYS:H	2.17	0.43
2:E:543:ILE:HG22	2:E:547:ILE:HG12	2.01	0.43
1:A:1076:THR:HA	1:A:1079:THR:HG22	2.00	0.43
2:D:548:ASN:OD1	2:D:549:LYS:N	2.48	0.43
1:A:989:ALA:HB1	1:A:1173:LEU:HD21	2.00	0.42
1:A:1257:LEU:HD23	1:A:1257:LEU:HA	1.87	0.42
2:C:519:GLY:O	2:C:523:SER:OG	2.34	0.42
1:A:1005:SER:HB2	1:A:1012:ILE:HG22	2.00	0.42
1:A:1253:ARG:HA	1:A:1413:THR:OG1	2.19	0.42
1:A:919:LEU:HD12	1:A:919:LEU:HA	1.85	0.42
2:D:538:GLU:O	2:D:541:LYS:HG2	2.19	0.42
1:A:350:ILE:HD11	1:A:1257:LEU:HD22	2.01	0.42
1:A:915:TRP:HA	1:A:915:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:LEU:HD12	1:A:1209:LEU:H	1.84	0.42
1:A:1236:CYS:SG	1:A:1239:CYS:HA	2.59	0.42
2:D:521:ILE:HG13	2:D:522:ASN:HD22	1.84	0.42
2:D:532:ARG:HD3	2:E:534:ASN:HD22	1.83	0.42
2:D:551:GLU:O	2:D:551:GLU:HG2	2.14	0.42
1:A:837:ALA:O	1:A:838:ILE:HG13	2.19	0.42
1:A:845:ASN:OD1	1:A:846:LEU:N	2.52	0.42
1:A:924:ARG:HH11	1:A:1169:GLN:NE2	2.17	0.42
1:A:138:THR:OG1	1:A:1229:TYR:HB2	2.19	0.42
1:A:252:VAL:HG23	1:A:258:TYR:HB3	2.01	0.42
1:A:817:SER:O	1:A:821:THR:HG23	2.20	0.42
1:A:1105:ALA:O	1:A:1109:MET:HG2	2.19	0.42
2:C:547:ILE:HD12	2:C:548:ASN:N	2.34	0.42
1:A:816:LEU:O	1:A:820:GLU:HG3	2.20	0.42
1:A:974:ASP:OD1	1:A:974:ASP:N	2.53	0.42
1:A:918:THR:OG1	1:A:919:LEU:N	2.53	0.42
1:A:1120:HIS:O	1:A:1121:GLU:HB3	2.19	0.42
1:A:1191:CYS:SG	1:A:1192:SER:N	2.92	0.42
2:D:541:LYS:O	2:D:544:PRO:HD2	2.20	0.42
1:A:1022:ASP:OD1	1:A:1023:LEU:N	2.53	0.42
1:A:1325:ARG:HD2	1:A:1325:ARG:HA	1.77	0.42
2:C:541:LYS:C	2:C:544:PRO:HD2	2.45	0.42
2:D:539:GLN:HE22	2:E:540:VAL:HG12	1.85	0.42
1:A:1226:VAL:O	1:A:1422:LEU:HB2	2.20	0.41
1:A:1080:ILE:HA	1:A:1080:ILE:HD12	1.75	0.41
1:A:1238:ILE:HB	1:A:1241:GLN:H	1.84	0.41
1:A:1250:PHE:HB3	1:A:1371:ASN:HB2	2.02	0.41
1:A:306:ILE:HD12	1:A:306:ILE:H	1.85	0.41
2:D:537:GLU:HA	2:D:540:VAL:HG22	2.02	0.41
2:E:568:GLU:HB3	2:E:570:HIS:CE1	2.54	0.41
1:A:423:HIS:CE1	2:B:559:LYS:HD2	2.55	0.41
1:A:501:GLU:H	1:A:501:GLU:CD	2.28	0.41
2:C:522:ASN:O	2:C:525:LYS:HG3	2.21	0.41
1:A:185:LYS:NZ	1:A:967:ILE:O	2.54	0.41
1:A:1156:PRO:HD2	1:A:1157:LYS:HZ3	1.85	0.41
2:D:536:ILE:O	2:D:540:VAL:HG22	2.20	0.41
2:D:703:ASP:HB2	2:D:708:ASN:HD21	1.86	0.41
1:A:37:HIS:ND1	1:A:39:GLN:HB2	2.35	0.41
1:A:289:MET:HE3	1:A:289:MET:HB3	1.86	0.41
1:A:1157:LYS:HE2	1:A:1157:LYS:H	1.85	0.41
1:A:261:LEU:HD22	1:A:261:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:HH21	2:D:699:ASN:HD22	1.69	0.41
1:A:867:ARG:NH2	2:D:576:ILE:O	2.54	0.41
1:A:376:LYS:HE2	1:A:376:LYS:HB2	1.80	0.41
1:A:803:GLN:O	1:A:807:THR:OG1	2.30	0.41
2:B:546:ILE:HB	2:C:547:ILE:HD13	2.02	0.41
1:A:8:SER:N	1:A:1146:ARG:HA	2.36	0.41
1:A:445:LYS:HE3	1:A:445:LYS:HB2	1.94	0.41
1:A:447:TRP:CD1	1:A:447:TRP:H	2.38	0.41
1:A:1256:GLN:HE21	1:A:1256:GLN:HB2	1.62	0.41
2:D:546:ILE:HB	2:E:547:ILE:HG21	2.03	0.41
2:D:557:LEU:O	2:D:560:THR:HG22	2.20	0.41
2:D:676:GLU:OE1	2:D:677:LEU:HD12	2.21	0.41
2:E:532:ARG:CA	2:E:535:HIS:HD1	2.34	0.41
1:A:556:MET:HE2	1:A:801:TYR:CE2	2.56	0.40
2:D:682:ILE:HG13	2:D:686:ASN:ND2	2.36	0.40
1:A:148:ILE:O	1:A:149:HIS:C	2.65	0.40
1:A:172:PHE:O	1:A:176:ILE:HG12	2.22	0.40
2:B:522:ASN:CB	2:B:525:LYS:HE3	2.50	0.40
1:A:306:ILE:HD11	1:A:853:GLU:HG3	2.03	0.40
1:A:830:GLN:HG2	1:A:834:GLU:HG2	2.02	0.40
2:E:531:MET:HE2	2:E:531:MET:HA	2.03	0.40
2:D:532:ARG:HD3	2:E:534:ASN:ND2	2.37	0.40
2:D:659:SER:O	2:D:663:VAL:HG23	2.21	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	1264/2244 (56%)	1181 (93%)	81 (6%)	2 (0%)	44 77
2	B	49/709 (7%)	43 (88%)	6 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	51/709 (7%)	43 (84%)	8 (16%)	0	100	100
2	D	113/709 (16%)	108 (96%)	4 (4%)	1 (1%)	14	49
2	E	52/709 (7%)	47 (90%)	5 (10%)	0	100	100
All	All	1529/5080 (30%)	1422 (93%)	104 (7%)	3 (0%)	45	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ILE
2	D	552	SER
1	A	922	GLU

### 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	1141/2046 (56%)	1048 (92%)	93 (8%)	9	34
2	B	47/625 (8%)	40 (85%)	7 (15%)	2	12
2	C	49/625 (8%)	41 (84%)	8 (16%)	2	9
2	D	107/625 (17%)	95 (89%)	12 (11%)	5	21
2	E	50/625 (8%)	45 (90%)	5 (10%)	6	25
All	All	1394/4546 (31%)	1269 (91%)	125 (9%)	10	30

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	60	SER
1	A	99	THR
1	A	137	ILE
1	A	138	THR
1	A	146	ILE
1	A	199	ILE

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Mol	Chain	Res	Type
1	A	231	THR
1	A	242	LEU
1	A	254	SER
1	A	256	ILE
1	A	261	LEU
1	A	263	SER
1	A	291	GLU
1	A	345	LEU
1	A	348	ASP
1	A	350	ILE
1	A	358	SER
1	A	367	ILE
1	A	381	MET
1	A	440	ILE
1	A	446	ASN
1	A	461	LEU
1	A	462	LYS
1	A	477	SER
1	A	481	ASP
1	A	482	GLU
1	A	489	ARG
1	A	495	THR
1	A	498	LYS
1	A	513	GLU
1	A	541	LEU
1	A	546	THR
1	A	556	MET
1	A	571	ILE
1	A	573	SER
1	A	575	VAL
1	A	714	THR
1	A	716	SER
1	A	720	THR
1	A	721	THR
1	A	728	LEU
1	A	748	LEU
1	A	761	ARG
1	A	776	ASP
1	A	781	LEU
1	A	787	ASP
1	A	789	ILE
1	A	830	GLN

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Mol	Chain	Res	Type
1	A	832	ASP
1	A	834	GLU
1	A	838	ILE
1	A	846	LEU
1	A	877	LEU
1	A	886	THR
1	A	901	VAL
1	A	904	GLN
1	A	917	GLU
1	A	918	THR
1	A	945	ASN
1	A	962	SER
1	A	975	VAL
1	A	983	LEU
1	A	1012	ILE
1	A	1020	LEU
1	A	1047	ASP
1	A	1080	ILE
1	A	1083	ASN
1	A	1095	ASP
1	A	1103	GLU
1	A	1127	LEU
1	A	1132	GLU
1	A	1138	LEU
1	A	1142	LYS
1	A	1159	VAL
1	A	1179	ASN
1	A	1186	ILE
1	A	1192	SER
1	A	1235	GLU
1	A	1253	ARG
1	A	1256	GLN
1	A	1259	GLN
1	A	1291	THR
1	A	1298	ILE
1	A	1311	ASN
1	A	1332	VAL
1	A	1364	ASN
1	A	1377	LEU
1	A	1381	ILE
1	A	1390	LEU
1	A	1394	GLN

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Mol	Chain	Res	Type
1	A	1401	SER
1	A	1440	ASP
2	B	528	ASN
2	B	536	ILE
2	B	538	GLU
2	B	547	ILE
2	B	548	ASN
2	B	554	ASP
2	B	561	ASN
2	C	520	VAL
2	C	523	SER
2	C	530	ASP
2	C	534	ASN
2	C	539	GLN
2	C	556	VAL
2	C	557	LEU
2	C	565	SER
2	D	528	ASN
2	D	545	LYS
2	D	550	LEU
2	D	551	GLU
2	D	556	VAL
2	D	560	THR
2	D	568	GLU
2	D	577	MET
2	D	660	SER
2	D	676	GLU
2	D	695	GLN
2	D	702	ASN
2	E	523	SER
2	E	536	ILE
2	E	541	LYS
2	E	551	GLU
2	E	568	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	79	ASN
1	A	213	ASN
1	A	349	ASN

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Mol	Chain	Res	Type
1	A	351	HIS
1	A	411	HIS
1	A	427	HIS
1	A	446	ASN
1	A	875	HIS
1	A	876	ASN
1	A	904	GLN
1	A	958	GLN
1	A	1000	ASN
1	A	1029	HIS
1	A	1038	GLN
1	A	1042	ASN
1	A	1169	GLN
1	A	1327	ASN
1	A	1394	GLN
1	A	1438	GLN
2	B	522	ASN
2	C	548	ASN
2	D	522	ASN
2	D	528	ASN
2	D	534	ASN
2	D	561	ASN
2	D	699	ASN
2	E	528	ASN
2	E	534	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

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	A1EF9	A	2301	-	38,39,39	4.05	19 (50%)	50,57,57	2.53	14 (28%)

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	A1EF9	A	2301	-	-	6/28/50/50	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2301	A1EF9	C26-C23	9.00	1.53	1.38
3	A	2301	A1EF9	C20-N10	-8.93	1.26	1.47
3	A	2301	A1EF9	C27-C23	8.71	1.52	1.38
3	A	2301	A1EF9	C28-C30	8.12	1.53	1.39
3	A	2301	A1EF9	C29-C30	8.02	1.52	1.39
3	A	2301	A1EF9	C28-C26	7.73	1.52	1.38
3	A	2301	A1EF9	C29-C27	7.65	1.52	1.38
3	A	2301	A1EF9	S01-N09	5.41	1.71	1.63
3	A	2301	A1EF9	C31-N11	3.59	1.45	1.35
3	A	2301	A1EF9	C23-S01	3.46	1.81	1.76
3	A	2301	A1EF9	C21-N10	-3.05	1.38	1.46
3	A	2301	A1EF9	C22-N10	-3.03	1.38	1.46
3	A	2301	A1EF9	C17-C15	-2.89	1.45	1.53
3	A	2301	A1EF9	O06-S01	2.76	1.46	1.43
3	A	2301	A1EF9	C33-C34	-2.62	1.36	1.39
3	A	2301	A1EF9	C18-N09	2.59	1.53	1.48
3	A	2301	A1EF9	O05-S01	2.57	1.46	1.43
3	A	2301	A1EF9	O08-C31	-2.26	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2301	A1EF9	C33-C32	-2.09	1.36	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2301	A1EF9	O06-S01-O05	-10.85	101.94	119.52
3	A	2301	A1EF9	C36-C34-N13	6.64	127.52	119.72
3	A	2301	A1EF9	C18-N09-C14	-6.36	107.95	116.10
3	A	2301	A1EF9	C34-N13-N12	5.05	108.16	104.37
3	A	2301	A1EF9	O05-S01-C23	3.16	112.05	108.05
3	A	2301	A1EF9	C33-C34-C36	-3.05	124.67	127.93
3	A	2301	A1EF9	O06-S01-N09	2.94	112.33	106.97
3	A	2301	A1EF9	O05-S01-N09	2.91	112.27	106.97
3	A	2301	A1EF9	C19-C18-N09	2.56	114.06	110.31
3	A	2301	A1EF9	C33-C34-N13	-2.49	107.80	111.41
3	A	2301	A1EF9	C16-C14-C15	-2.20	109.22	112.58
3	A	2301	A1EF9	F04-C36-C34	-2.16	108.78	112.47
3	A	2301	A1EF9	C33-C32-C31	-2.15	121.86	128.55
3	A	2301	A1EF9	C15-C14-N09	2.11	113.16	109.50

There are no chirality outliers.

All (6) torsion outliers are listed below:

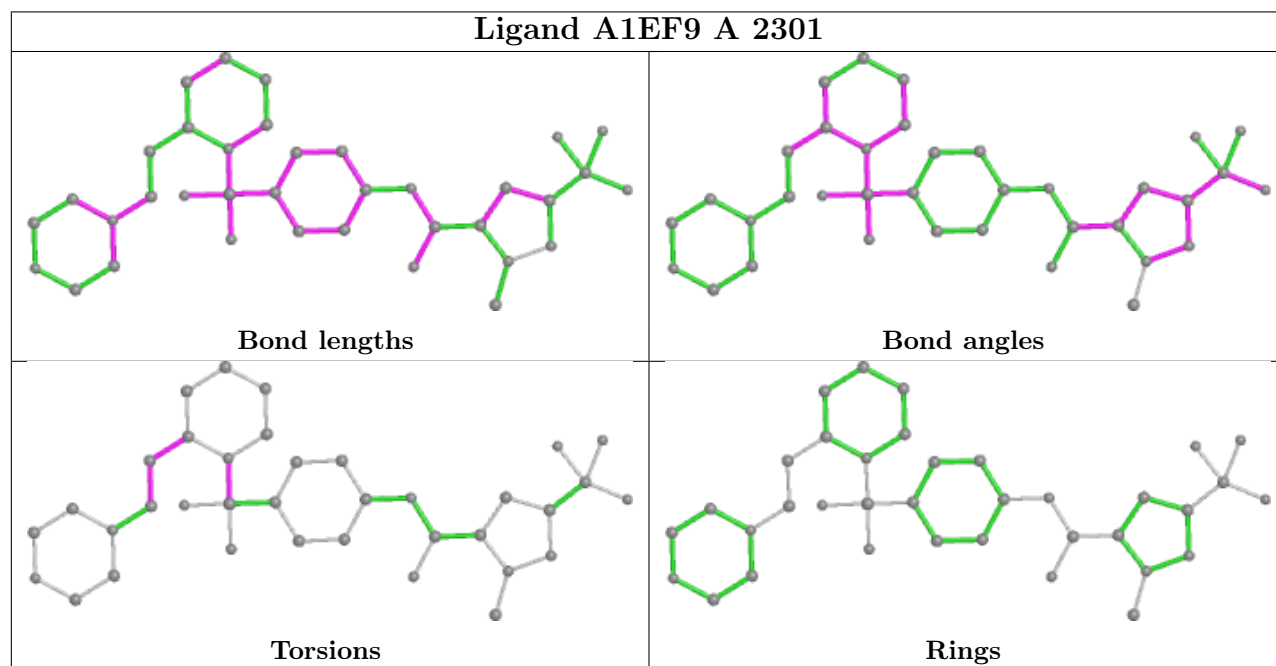
Mol	Chain	Res	Type	Atoms
3	A	2301	A1EF9	C14-C16-C20-N10
3	A	2301	A1EF9	C18-N09-S01-C23
3	A	2301	A1EF9	C18-N09-S01-O06
3	A	2301	A1EF9	N09-C14-C16-C20
3	A	2301	A1EF9	C15-C14-C16-C20
3	A	2301	A1EF9	C14-N09-S01-O06

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.