



## Full wwPDB EM Validation Report ⓘ

Sep 14, 2025 – 12:16 AM JST

PDB ID : 9KNV / pdb\_00009knv  
EMDB ID : EMD-62463  
Title : AS-136A-bound measles virus L-P complex  
Authors : Wang, Y.R.; Zhang, H.Q.  
Deposited on : 2024-11-19  
Resolution : 3.30 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

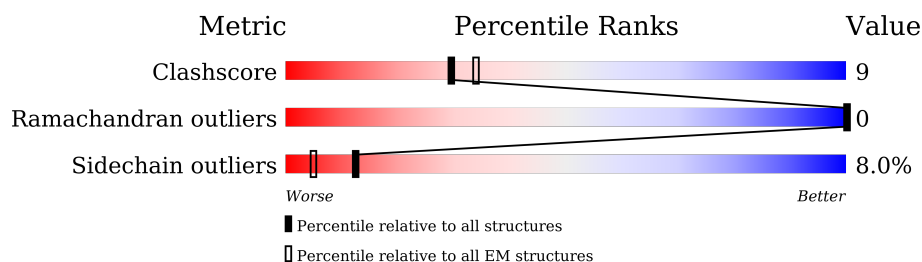
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	2183	
2	B	507	
2	C	507	
2	D	507	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11528 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	1275	Total	C	N	O	S	0	0
			10241	6535	1771	1876	59		

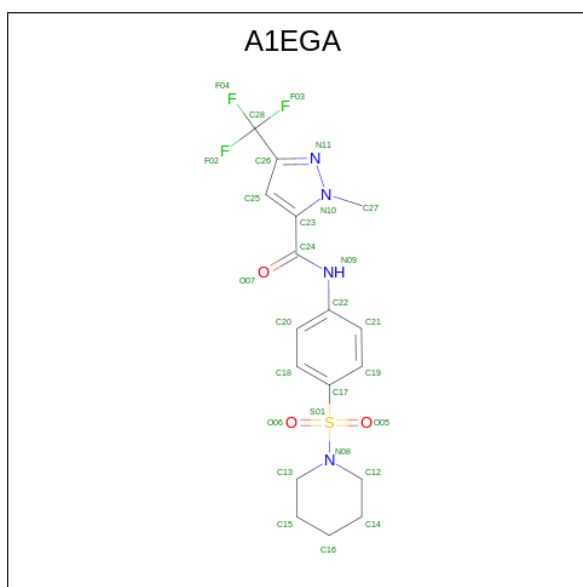
- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	28	Total	C	N	O	S	0	0
			207	129	37	40	1		
2	D	41	Total	C	N	O	S	0	0
			305	188	53	63	1		
2	C	95	Total	C	N	O	S	0	0
			745	476	133	132	4		

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

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

- Molecule 4 is 2-methyl- {N}-(4-piperidin-1-ylsulfonylphenyl)-5-(trifluoromethyl)pyrazole-3-carboxamide (CCD ID: A1EGA) (formula: C<sub>17</sub>H<sub>19</sub>F<sub>3</sub>N<sub>4</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).

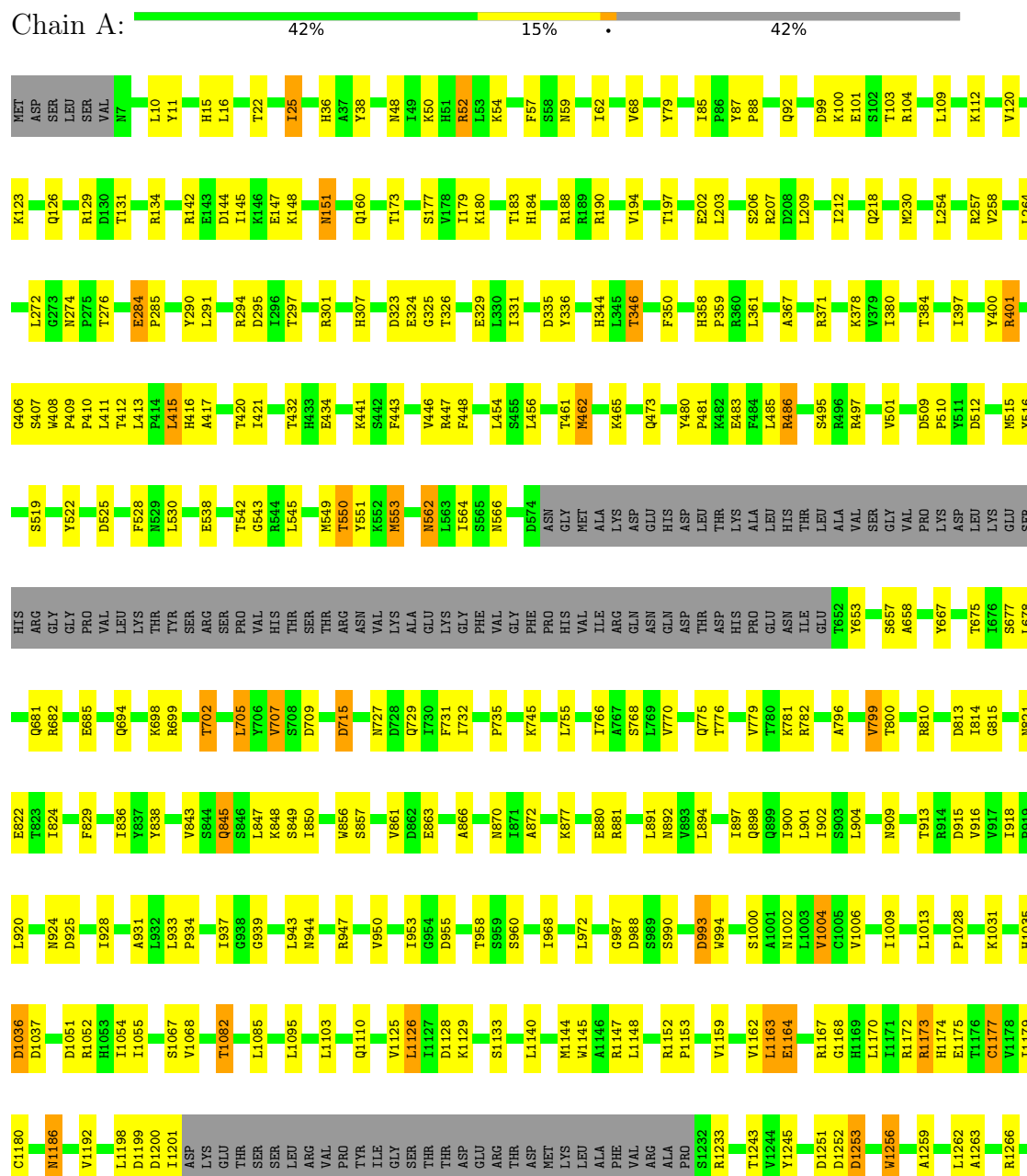


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	28	17	3	4	3	1	0

### 3 Residue-property plots [i](#)

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











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126133	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: ZN, A1EGA

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	0/10470	0.35	0/14193
2	B	0.12	0/208	0.28	0/279
2	C	0.14	0/753	0.34	0/1001
2	D	0.14	0/309	0.41	0/421
All	All	0.17	0/11740	0.35	0/15894

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	10241	0	10251	191	0
2	B	207	0	218	6	0
2	C	745	0	812	14	0
2	D	305	0	305	7	0
3	A	2	0	0	0	0
4	A	28	0	0	0	0
All	All	11528	0	11586	209	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 9.

All (209) 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:284:GLU:HG3	1:A:285:PRO:HD3	1.55	0.87
1:A:658:ALA:HB3	1:A:800:THR:HG21	1.65	0.78
1:A:257:ARG:NH1	1:A:336:TYR:O	2.20	0.74
1:A:408:TRP:HB3	1:A:411:LEU:HB2	1.71	0.73
1:A:1253:ASP:N	1:A:1253:ASP:OD1	2.22	0.72
1:A:378:LYS:NZ	1:A:815:GLY:O	2.23	0.72
1:A:1186:ASN:N	1:A:1186:ASN:OD1	2.25	0.69
1:A:401:ARG:HG3	1:A:406:GLY:HA2	1.74	0.69
1:A:768:SER:OG	1:A:775:GLN:NE2	2.27	0.67
1:A:384:THR:HG21	1:A:813:ASP:HB3	1.75	0.67
1:A:1180:CYS:SG	1:A:1364:HIS:NE2	2.67	0.66
1:A:441:LYS:NZ	2:B:364:GLU:OE2	2.29	0.66
1:A:681:GLN:NE2	1:A:685:GLU:OE2	2.29	0.65
1:A:15:HIS:NE2	1:A:856:TRP:O	2.29	0.64
1:A:1307:VAL:O	1:A:1311:THR:OG1	2.14	0.64
1:A:1167:ARG:NH1	1:A:1366:GLU:OE2	2.31	0.64
1:A:112:LYS:NZ	1:A:924:ASN:OD1	2.31	0.63
1:A:1036:ASP:N	1:A:1036:ASP:OD1	2.31	0.63
1:A:653:TYR:O	1:A:782:ARG:NH2	2.32	0.63
1:A:1192:VAL:HG23	1:A:1310:TYR:HB3	1.79	0.63
1:A:400:TYR:HE2	1:A:409:PRO:HD2	1.64	0.62
1:A:417:ALA:HB1	1:A:421:ILE:HG23	1.80	0.62
2:B:371:MET:HB2	2:C:397:ILE:HG12	1.80	0.62
1:A:715:ASP:OD1	1:A:729:GLN:NE2	2.32	0.62
1:A:380:ILE:HD11	2:B:372:ILE:HD12	1.80	0.61
1:A:432:THR:HG23	1:A:434:GLU:H	1.65	0.61
1:A:1031:LYS:O	1:A:1395:ASN:ND2	2.33	0.61
1:A:990:SER:OG	1:A:993:ASP:OD1	2.19	0.61
1:A:1002:ASN:OD1	1:A:1145:TRP:NE1	2.25	0.60
2:C:401:ASP:HB2	2:C:404:ARG:HG3	1.83	0.60
1:A:705:LEU:HD11	1:A:735:PRO:HG3	1.84	0.60
1:A:79:TYR:OH	1:A:202:GLU:OE2	2.16	0.59
1:A:184:HIS:O	1:A:188:ARG:NH2	2.35	0.59
1:A:955:ASP:HB3	1:A:958:THR:HG22	1.84	0.59
1:A:1173:ARG:NH2	1:A:1174:HIS:O	2.35	0.59
1:A:416:HIS:CE1	2:D:362:THR:HA	2.37	0.59
1:A:123:LYS:HB2	1:A:972:LEU:HD13	1.85	0.57
1:A:987:GLY:HA2	1:A:1004:VAL:HG13	1.85	0.57
1:A:101:GLU:HG3	1:A:104:ARG:HH21	1.69	0.57
1:A:1274:LEU:O	1:A:1278:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:LEU:HG	2:D:373:ALA:HB2	1.88	0.55
2:C:487:ASP:OD1	2:C:487:ASP:N	2.39	0.55
1:A:367:ALA:HB2	1:A:707:VAL:HG11	1.89	0.55
1:A:131:THR:HG23	1:A:1163:LEU:HD21	1.88	0.55
2:C:479:ARG:O	2:C:483:THR:HG23	2.07	0.54
1:A:1198:LEU:HD23	1:A:1306:ARG:HD2	1.88	0.54
2:C:485:LEU:HD12	2:C:497:PHE:HE2	1.72	0.54
1:A:57:PHE:HE2	1:A:483:GLU:HG3	1.72	0.54
1:A:781:LYS:HD2	1:A:799:VAL:HG21	1.90	0.54
1:A:11:TYR:HE1	1:A:180:LYS:HE3	1.73	0.53
1:A:1028:PRO:HA	1:A:1031:LYS:HG2	1.90	0.53
1:A:52:ARG:HG3	1:A:57:PHE:HB3	1.90	0.53
1:A:134:ARG:NH1	1:A:1164:GLU:O	2.41	0.53
1:A:933:LEU:HB3	1:A:939:GLY:HA3	1.91	0.53
1:A:456:LEU:HD11	1:A:510:PRO:HB2	1.91	0.52
1:A:371:ARG:NH1	1:A:727:ASN:OD1	2.42	0.52
1:A:677:SER:OG	2:D:372:ILE:O	2.20	0.52
1:A:1321:VAL:HG12	1:A:1322:ILE:H	1.75	0.52
1:A:16:LEU:HD22	1:A:230:MET:HB2	1.91	0.52
1:A:1263:ALA:HB3	1:A:1274:LEU:HD11	1.90	0.52
1:A:206:SER:OG	1:A:207:ARG:N	2.43	0.52
1:A:291:LEU:HD13	1:A:346:THR:HG21	1.91	0.52
1:A:1051:ASP:OD2	1:A:1384:ARG:NH1	2.43	0.52
1:A:203:LEU:HD23	1:A:212:ILE:HG12	1.92	0.51
1:A:36:HIS:HD2	1:A:38:TYR:HB2	1.76	0.51
1:A:1067:SER:OG	1:A:1068:VAL:N	2.43	0.51
1:A:380:ILE:HG12	2:B:372:ILE:HB	1.93	0.51
1:A:1052:ARG:O	1:A:1152:ARG:NH1	2.42	0.51
1:A:1082:THR:HG23	1:A:1085:LEU:H	1.76	0.51
1:A:1199:ASP:OD1	1:A:1200:ASP:N	2.43	0.51
2:C:492:ASN:O	2:C:496:LYS:HG2	2.12	0.50
1:A:913:THR:OG1	1:A:915:ASP:OD1	2.21	0.50
1:A:1252:ASP:H	1:A:1256:TRP:CD1	2.29	0.50
1:A:344:HIS:HA	1:A:843:VAL:HG12	1.94	0.49
1:A:904:LEU:HD11	1:A:920:LEU:HD13	1.92	0.49
1:A:495:SER:HB2	1:A:501:VAL:HG22	1.94	0.49
1:A:99:ASP:OD1	1:A:100:LYS:N	2.45	0.49
1:A:325:GLY:O	1:A:329:GLU:HG3	2.12	0.49
1:A:409:PRO:HB2	1:A:410:PRO:HD3	1.95	0.49
1:A:1385:LYS:HD2	1:A:1386:LEU:H	1.78	0.49
2:C:459:ALA:O	2:C:463:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:HD11	1:A:412:THR:HG23	1.95	0.48
1:A:894:LEU:O	1:A:898:GLN:HG2	2.13	0.48
1:A:1343:VAL:HA	1:A:1346:THR:HG22	1.94	0.48
1:A:291:LEU:HD12	1:A:294:ARG:HE	1.78	0.48
1:A:1054:ILE:HG12	1:A:1153:PRO:HG2	1.94	0.48
2:C:460:SER:O	2:C:464:ILE:HG13	2.13	0.48
1:A:480:TYR:HB2	1:A:485:LEU:HD11	1.95	0.48
1:A:950:VAL:HG11	1:A:1162:VAL:HG11	1.94	0.48
1:A:407:SER:C	1:A:408:TRP:HD1	2.22	0.48
1:A:1200:ASP:OD1	1:A:1201:ILE:N	2.41	0.48
1:A:1173:ARG:NE	1:A:1174:HIS:H	2.12	0.47
1:A:50:LYS:O	1:A:54:LYS:HG2	2.13	0.47
1:A:1145:TRP:CE3	1:A:1147:ARG:HB3	2.49	0.47
1:A:461:THR:O	1:A:465:LYS:HG2	2.15	0.47
1:A:1002:ASN:HB3	1:A:1145:TRP:CD1	2.50	0.47
2:B:364:GLU:HB2	2:D:363:LEU:HG	1.96	0.47
2:D:352:GLN:HA	2:D:355:ARG:HH21	1.79	0.47
1:A:179:ILE:O	1:A:183:THR:HG23	2.14	0.47
1:A:144:ASP:O	1:A:148:LYS:HG2	2.14	0.47
2:C:455:ASP:OD2	2:C:456:THR:N	2.43	0.47
1:A:1245:TYR:OH	1:A:1259:ALA:HA	2.15	0.46
1:A:454:LEU:HD13	2:D:390:LEU:HD21	1.96	0.46
1:A:550:THR:HG22	1:A:551:TYR:H	1.80	0.46
1:A:562:ASN:OD1	1:A:566:ASN:ND2	2.48	0.46
1:A:900:ILE:HD12	1:A:931:ALA:HB2	1.96	0.46
1:A:1245:TYR:CZ	1:A:1262:LEU:HB2	2.51	0.46
1:A:407:SER:C	1:A:409:PRO:HD3	2.40	0.46
1:A:755:LEU:HB3	1:A:766:ILE:HD11	1.98	0.46
2:C:483:THR:HA	2:C:486:ASP:OD2	2.16	0.46
1:A:836:ILE:HB	1:A:843:VAL:HG23	1.98	0.46
1:A:1051:ASP:OD1	1:A:1152:ARG:NH1	2.31	0.46
1:A:1173:ARG:H	1:A:1173:ARG:HG3	1.37	0.46
1:A:1179:ILE:HG23	1:A:1364:HIS:CE1	2.51	0.46
1:A:448:PHE:HD2	1:A:682:ARG:HD3	1.80	0.46
1:A:821:ASN:HB3	1:A:822:GLU:OE1	2.16	0.45
1:A:1140:LEU:O	1:A:1144:MET:HB2	2.16	0.45
1:A:497:ARG:O	1:A:501:VAL:HG23	2.16	0.45
1:A:25:ILE:H	1:A:25:ILE:HG13	1.59	0.45
1:A:872:ALA:HB1	1:A:943:LEU:HB2	1.99	0.45
1:A:1372:ILE:HG23	1:A:1374:MET:HE3	1.98	0.45
1:A:371:ARG:NH1	1:A:731:PHE:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:OD1	1:A:486:ARG:NH1	2.49	0.45
1:A:934:PRO:HB2	1:A:960:SER:HB3	1.99	0.45
1:A:1266:ARG:O	1:A:1399:TYR:HB2	2.16	0.45
1:A:564:ILE:HG23	1:A:745:LYS:HB2	1.99	0.45
1:A:522:TYR:HB2	1:A:553:MET:HE2	1.99	0.44
1:A:516:TYR:OH	1:A:525:ASP:OD2	2.27	0.44
1:A:1145:TRP:CZ3	1:A:1147:ARG:HB3	2.53	0.44
1:A:147:GLU:OE1	1:A:151:ASN:ND2	2.51	0.44
1:A:151:ASN:OD1	1:A:151:ASN:N	2.50	0.44
1:A:1180:CYS:SG	1:A:1362:HIS:ND1	2.91	0.44
1:A:968:ILE:HG22	1:A:1129:LYS:HD3	2.00	0.44
1:A:11:TYR:CE1	1:A:180:LYS:HE3	2.53	0.44
1:A:694:GLN:HG3	1:A:698:LYS:HD2	1.98	0.44
1:A:947:ARG:HA	1:A:947:ARG:HD2	1.84	0.44
1:A:1302:THR:O	1:A:1302:THR:OG1	2.26	0.44
1:A:1145:TRP:CE3	1:A:1148:LEU:HG	2.53	0.44
1:A:528:PHE:HB3	1:A:699:ARG:HH21	1.83	0.43
2:C:393:ASP:O	2:C:394:LEU:HD23	2.18	0.43
1:A:359:PRO:HD2	1:A:538:GLU:O	2.17	0.43
1:A:515:MET:O	1:A:519:SER:OG	2.26	0.43
1:A:1332:ILE:HB	1:A:1335:GLN:HG2	2.00	0.43
1:A:1362:HIS:HB3	1:A:1364:HIS:CE1	2.53	0.43
1:A:190:ARG:HA	1:A:190:ARG:NH1	2.33	0.43
1:A:290:TYR:OH	1:A:335:ASP:OD1	2.37	0.43
1:A:916:VAL:O	1:A:920:LEU:HB2	2.18	0.43
1:A:1256:TRP:CZ3	1:A:1274:LEU:HD22	2.53	0.43
1:A:447:ARG:HE	1:A:447:ARG:HB3	1.60	0.43
1:A:142:ARG:HB2	1:A:145:ILE:HG13	2.01	0.43
1:A:549:MET:SD	1:A:553:MET:HB3	2.59	0.43
1:A:845:GLN:NE2	1:A:848:LYS:HD2	2.33	0.43
1:A:542:THR:OG1	1:A:543:GLY:N	2.52	0.43
1:A:68:VAL:HG11	1:A:209:LEU:HD21	2.01	0.43
1:A:254:LEU:O	1:A:258:VAL:HG23	2.19	0.43
1:A:796:ALA:O	1:A:800:THR:HG23	2.19	0.43
1:A:810:ARG:O	1:A:814:ILE:HG23	2.19	0.43
1:A:509:ASP:HB3	1:A:512:ASP:HB2	2.00	0.42
1:A:11:TYR:CE2	1:A:861:VAL:HG13	2.54	0.42
1:A:415:LEU:H	1:A:415:LEU:HD23	1.85	0.42
1:A:857:SER:HB2	1:A:870:ASN:HB3	2.01	0.42
1:A:1177:CYS:HB2	1:A:1180:CYS:HB2	2.01	0.42
1:A:877:LYS:HB2	1:A:877:LYS:HE3	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.90	0.42
1:A:925:ASP:O	1:A:928:ILE:HG12	2.20	0.42
2:C:468:ILE:O	2:C:471:SER:OG	2.37	0.42
1:A:1167:ARG:HB2	1:A:1167:ARG:HH11	1.85	0.42
2:C:503:LYS:HB3	2:C:503:LYS:HE2	1.74	0.42
1:A:11:TYR:OH	1:A:909:ASN:OD1	2.38	0.41
1:A:473:GLN:HB2	1:A:528:PHE:O	2.19	0.41
1:A:847:LEU:HD23	1:A:850:ILE:HD12	2.02	0.41
1:A:295:ASP:O	1:A:301:ARG:NH2	2.52	0.41
1:A:944:ASN:HD21	1:A:953:ILE:HD13	1.85	0.41
1:A:1273:GLU:HA	1:A:1276:VAL:HG22	2.01	0.41
1:A:87:TYR:OH	1:A:358:HIS:O	2.31	0.41
1:A:126:GLN:OE1	1:A:129:ARG:NH2	2.54	0.41
2:D:368:SER:O	2:D:372:ILE:HG12	2.20	0.41
1:A:1000:SER:O	1:A:1000:SER:OG	2.30	0.41
1:A:1170:LEU:HD11	1:A:1347:LEU:HD22	2.02	0.41
1:A:297:THR:O	1:A:297:THR:OG1	2.37	0.41
1:A:462:MET:H	1:A:462:MET:HG2	1.53	0.41
1:A:845:GLN:O	1:A:881:ARG:HD3	2.20	0.41
1:A:988:ASP:HA	1:A:1145:TRP:HZ2	1.86	0.41
1:A:1035:HIS:HB2	1:A:1037:ASP:OD1	2.20	0.41
1:A:1363:LEU:HD12	1:A:1363:LEU:HA	1.90	0.41
1:A:421:ILE:HD11	1:A:443:PHE:CZ	2.56	0.41
1:A:779:VAL:HB	1:A:800:THR:HG22	2.03	0.41
1:A:877:LYS:O	1:A:880:GLU:HG2	2.21	0.41
1:A:915:ASP:OD1	1:A:915:ASP:N	2.53	0.41
1:A:918:ILE:HD13	1:A:918:ILE:HA	1.91	0.41
1:A:1252:ASP:OD1	1:A:1379:ARG:HG2	2.21	0.41
1:A:59:ASN:OD1	1:A:62:ILE:HG12	2.20	0.41
1:A:994:TRP:HZ3	1:A:1145:TRP:CD1	2.39	0.41
1:A:1009:ILE:HG23	1:A:1103:LEU:HD22	2.03	0.41
1:A:1013:LEU:HD12	1:A:1013:LEU:HA	1.87	0.41
1:A:1125:VAL:HG13	1:A:1126:LEU:HD22	2.03	0.41
1:A:1167:ARG:HG2	1:A:1168:GLY:H	1.86	0.41
1:A:87:TYR:CE1	1:A:230:MET:HE1	2.56	0.40
1:A:307:HIS:HB3	1:A:821:ASN:ND2	2.36	0.40
1:A:481:PRO:HB2	1:A:483:GLU:OE2	2.20	0.40
1:A:702:THR:O	1:A:702:THR:OG1	2.29	0.40
2:B:377:LEU:HD23	2:B:377:LEU:HA	1.91	0.40
2:C:469:LYS:HB2	2:C:469:LYS:HE3	1.69	0.40
1:A:88:PRO:HG2	1:A:274:ASN:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:OD2	1:A:324:GLU:N	2.53	0.40
1:A:829:PHE:HB3	1:A:838:TYR:CD2	2.56	0.40
1:A:1172:ARG:N	1:A:1175:GLU:OE2	2.40	0.40
1:A:1354:THR:O	1:A:1354:THR:OG1	2.31	0.40
1:A:863:GLU:HG3	1:A:866:ALA:HB3	2.03	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	1267/2183 (58%)	1198 (95%)	69 (5%)	0	100	100
2	B	26/507 (5%)	26 (100%)	0	0	100	100
2	C	91/507 (18%)	88 (97%)	3 (3%)	0	100	100
2	D	39/507 (8%)	34 (87%)	5 (13%)	0	100	100
All	All	1423/3704 (38%)	1346 (95%)	77 (5%)	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	1137/1945 (58%)	1045 (92%)	92 (8%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	24/416 (6%)	22 (92%)	2 (8%)	9	31
2	C	83/416 (20%)	79 (95%)	4 (5%)	21	50
2	D	36/416 (9%)	31 (86%)	5 (14%)	3	13
All	All	1280/3193 (40%)	1177 (92%)	103 (8%)	12	32

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	22	THR
1	A	25	ILE
1	A	52	ARG
1	A	85	ILE
1	A	92	GLN
1	A	103	THR
1	A	109	LEU
1	A	120	VAL
1	A	151	ASN
1	A	160	GLN
1	A	173	THR
1	A	177	SER
1	A	194	VAL
1	A	197	THR
1	A	218	GLN
1	A	264	LEU
1	A	276	THR
1	A	284	GLU
1	A	326	THR
1	A	331	ILE
1	A	346	THR
1	A	350	PHE
1	A	361	LEU
1	A	401	ARG
1	A	413	LEU
1	A	415	LEU
1	A	420	THR
1	A	446	VAL
1	A	462	MET
1	A	486	ARG
1	A	530	LEU
1	A	545	LEU

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Mol	Chain	Res	Type
1	A	550	THR
1	A	553	MET
1	A	562	ASN
1	A	657	SER
1	A	667	TYR
1	A	675	THR
1	A	702	THR
1	A	705	LEU
1	A	707	VAL
1	A	709	ASP
1	A	715	ASP
1	A	732	ILE
1	A	770	VAL
1	A	776	THR
1	A	799	VAL
1	A	824	ILE
1	A	845	GLN
1	A	849	SER
1	A	891	LEU
1	A	892	ASN
1	A	897	ILE
1	A	901	LEU
1	A	902	ILE
1	A	937	ILE
1	A	993	ASP
1	A	1004	VAL
1	A	1006	VAL
1	A	1036	ASP
1	A	1055	ILE
1	A	1082	THR
1	A	1095	LEU
1	A	1110	GLN
1	A	1126	LEU
1	A	1128	ASP
1	A	1133	SER
1	A	1159	VAL
1	A	1163	LEU
1	A	1164	GLU
1	A	1173	ARG
1	A	1177	CYS
1	A	1186	ASN
1	A	1233	ARG

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Mol	Chain	Res	Type
1	A	1243	THR
1	A	1251	ASP
1	A	1253	ASP
1	A	1256	TRP
1	A	1269	VAL
1	A	1273	GLU
1	A	1280	ILE
1	A	1310	TYR
1	A	1313	ILE
1	A	1321	VAL
1	A	1332	ILE
1	A	1354	THR
1	A	1359	THR
1	A	1365	VAL
1	A	1372	ILE
1	A	1375	ILE
1	A	1392	LEU
2	B	355	ARG
2	B	363	LEU
2	D	353	ILE
2	D	356	GLN
2	D	357	ASN
2	D	370	ILE
2	D	390	LEU
2	C	397	ILE
2	C	408	GLU
2	C	453	VAL
2	C	471	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	36	HIS
1	A	91	ASN
1	A	114	ASN
1	A	132	ASN
1	A	292	GLN
1	A	376	GLN
1	A	398	ASN
1	A	425	GLN
1	A	473	GLN

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Mol	Chain	Res	Type
1	A	697	HIS
1	A	775	GLN
1	A	816	HIS
1	A	817	HIS
1	A	821	ASN
1	A	845	GLN
1	A	899	GLN
1	A	1007	GLN
1	A	1401	ASN
2	D	357	ASN
2	D	366	HIS

### 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 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	A1EGA	A	2203	-	29,30,30	4.27	16 (55%)	40,45,45	3.23	15 (37%)

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	A1EGA	A	2203	-	-	9/23/34/34	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2203	A1EGA	C18-C17	8.76	1.52	1.38
4	A	2203	A1EGA	C19-C17	8.70	1.52	1.38
4	A	2203	A1EGA	C21-C22	7.97	1.52	1.39
4	A	2203	A1EGA	C20-C22	7.80	1.52	1.39
4	A	2203	A1EGA	C18-C20	7.66	1.52	1.38
4	A	2203	A1EGA	C19-C21	7.42	1.52	1.38
4	A	2203	A1EGA	S01-N08	5.24	1.70	1.63
4	A	2203	A1EGA	C12-N08	4.61	1.52	1.47
4	A	2203	A1EGA	C13-N08	4.59	1.52	1.47
4	A	2203	A1EGA	C24-N09	3.19	1.44	1.35
4	A	2203	A1EGA	C25-C26	-3.08	1.35	1.39
4	A	2203	A1EGA	C17-S01	2.96	1.80	1.76
4	A	2203	A1EGA	O06-S01	2.63	1.46	1.43
4	A	2203	A1EGA	O05-S01	2.55	1.46	1.43
4	A	2203	A1EGA	O07-C24	-2.41	1.18	1.23
4	A	2203	A1EGA	C25-C23	-2.37	1.36	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2203	A1EGA	O06-S01-O05	-10.75	102.10	119.52
4	A	2203	A1EGA	C28-C26-N11	7.42	128.44	119.72
4	A	2203	A1EGA	C22-N09-C24	-7.02	108.35	126.58
4	A	2203	A1EGA	O05-S01-N08	6.50	112.62	106.69
4	A	2203	A1EGA	O06-S01-N08	5.84	112.02	106.69
4	A	2203	A1EGA	C26-N11-N10	4.88	108.03	104.37
4	A	2203	A1EGA	C25-C26-C28	-4.16	123.49	127.93
4	A	2203	A1EGA	O06-S01-C17	3.21	112.11	108.05
4	A	2203	A1EGA	C12-N08-C13	-3.06	108.78	112.17
4	A	2203	A1EGA	O07-C24-N09	-3.06	116.72	123.71
4	A	2203	A1EGA	C13-N08-S01	2.70	121.96	117.05
4	A	2203	A1EGA	C12-N08-S01	2.31	121.24	117.05
4	A	2203	A1EGA	C25-C26-N11	-2.30	108.07	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2203	A1EGA	C25-C23-C24	-2.30	121.38	128.55
4	A	2203	A1EGA	F02-C28-C26	-2.29	108.55	112.47

There are no chirality outliers.

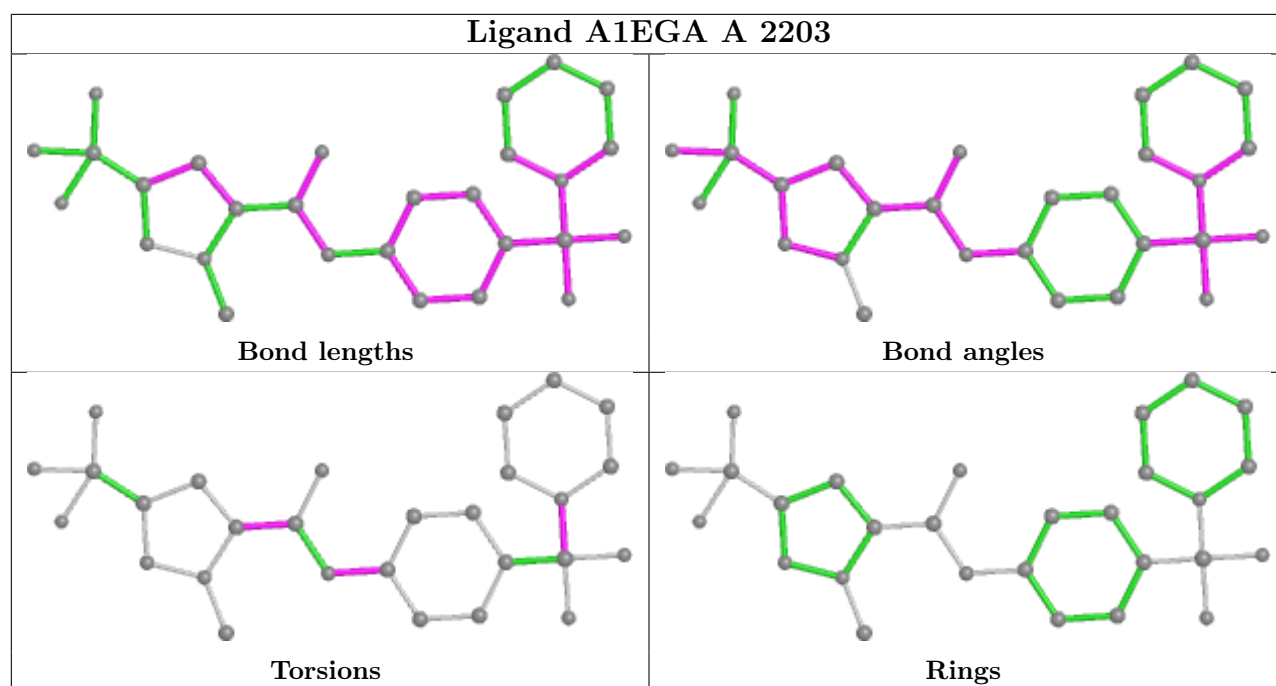
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2203	A1EGA	C13-N08-S01-O06
4	A	2203	A1EGA	C12-N08-S01-O05
4	A	2203	A1EGA	C13-N08-S01-C17
4	A	2203	A1EGA	C20-C22-N09-C24
4	A	2203	A1EGA	C21-C22-N09-C24
4	A	2203	A1EGA	C13-N08-S01-O05
4	A	2203	A1EGA	C12-N08-S01-C17
4	A	2203	A1EGA	C12-N08-S01-O06
4	A	2203	A1EGA	C25-C23-C24-O07

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.