



Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 02:30 AM JST

PDB ID : 9J8V / pdb_00009j8v
EMDB ID : EMD-61241
Title : TSWV L protein in complex with ribavirin 5-triphosphate
Authors : Cao, L.; Wang, X.
Deposited on : 2024-08-21
Resolution : 3.10 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 Phenix2.0rc1
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) : 2.44

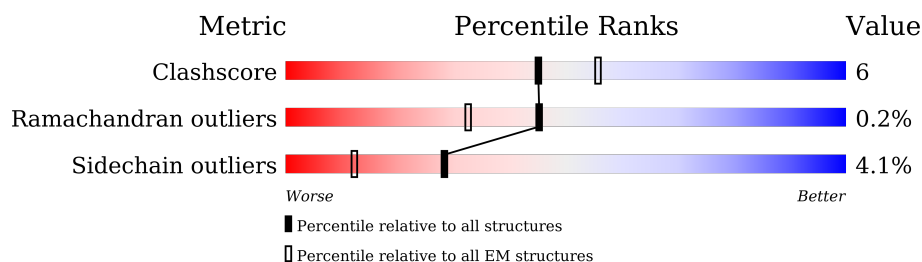
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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 ≥ 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	1766	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13498 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.

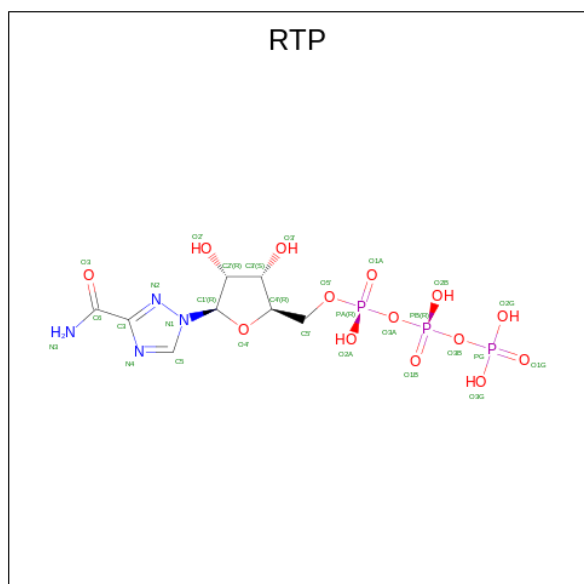
- Molecule 1 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1677	Total	C	N	O	S	0	0
			13440	8564	2218	2564	94		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1794	ALA	-	insertion	UNP A0A7G8JUQ9
A	1866	ALA	GLU	conflict	UNP A0A7G8JUQ9
A	1888	GLU	VAL	conflict	UNP A0A7G8JUQ9
A	1984	GLY	CYS	conflict	UNP A0A7G8JUQ9

- Molecule 2 is RIBAVIRIN TRIPHOSPHATE (CCD ID: RTP) (formula: $C_8H_{15}N_4O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



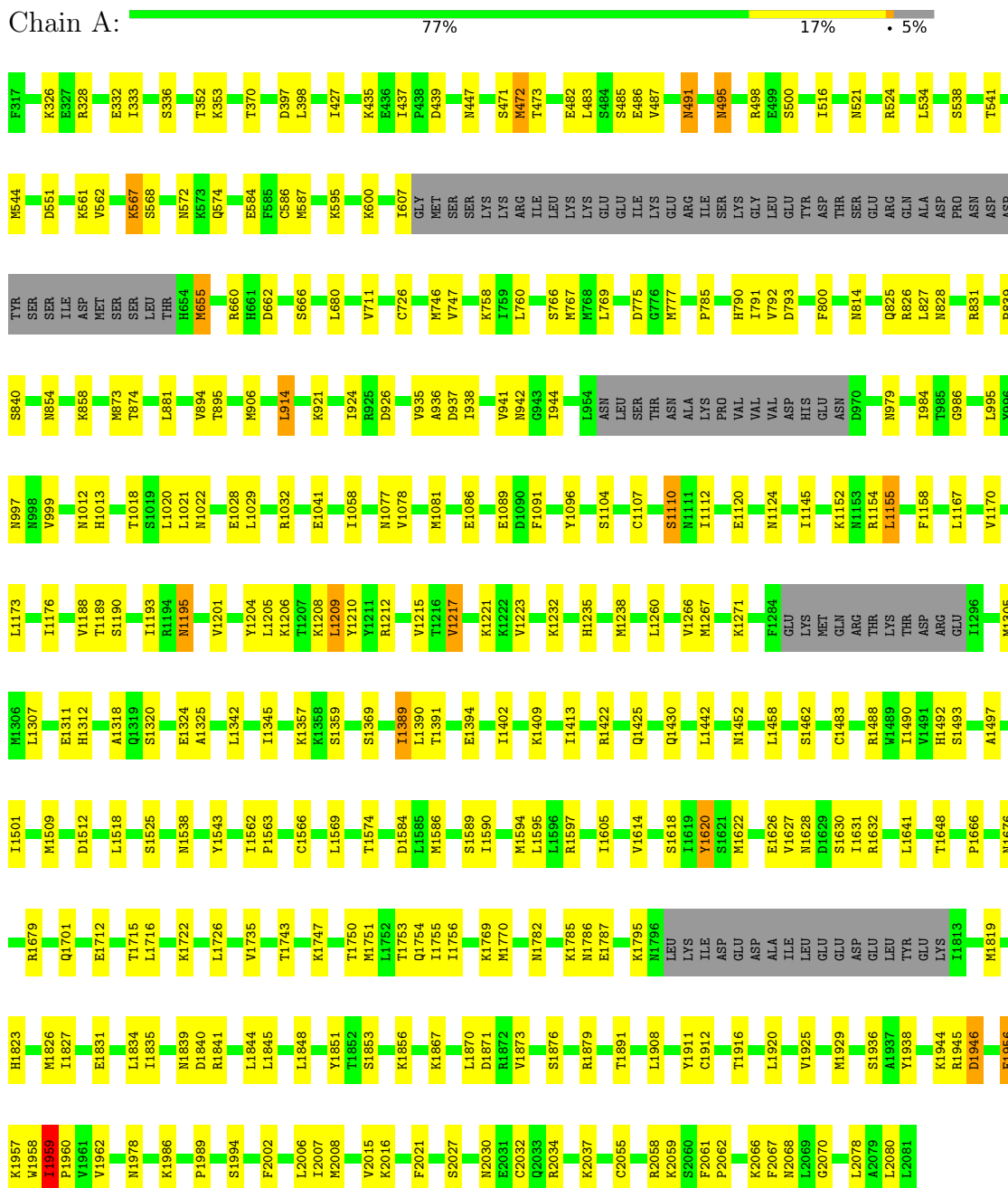
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	29	8	4	14	3	0

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144209	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RTP

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	0.22	0/13684	0.55	5/18440 (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	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2066	LYS	CA-CB-CG	6.62	127.33	114.10
1	A	1908	LEU	CA-C-N	5.53	132.44	123.93
1	A	1908	LEU	C-N-CA	5.53	132.44	123.93
1	A	486	GLU	CA-CB-CG	5.43	124.96	114.10
1	A	1389	ILE	CA-CB-CG1	5.31	119.43	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1962	VAL	Peptide
1	A	936	ALA	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	13440	0	13503	163	0
2	A	58	0	22	3	0
All	All	13498	0	13525	165	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 6.

All (165) 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:A:2101:RTP:O4'	2:A:2101:RTP:C4'	1.63	1.19
2:A:2102:RTP:C4'	2:A:2102:RTP:O4'	1.63	1.12
1:A:1589:SER:HB2	1:A:1666:PRO:HB3	1.75	0.68
1:A:1307:LEU:O	1:A:1311:GLU:HB2	1.94	0.66
1:A:938:ILE:O	1:A:942:ASN:HB2	1.96	0.65
1:A:1018:THR:O	1:A:1022:ASN:HB2	1.98	0.63
1:A:1318:ALA:HB1	1:A:1324:GLU:HG2	1.81	0.61
1:A:1369:SER:HB3	1:A:1538:ASN:HB2	1.83	0.61
1:A:941:VAL:HA	1:A:944:ILE:HD12	1.84	0.60
1:A:984:ILE:HD12	1:A:986:GLY:H	1.65	0.60
1:A:1154:ARG:HH11	1:A:1212:ARG:HE	1.48	0.60
1:A:1614:VAL:O	1:A:1618:SER:HB3	2.02	0.60
1:A:1782:ASN:HA	1:A:1785:LYS:HB3	1.83	0.59
1:A:2068:ASN:ND2	1:A:2070:GLY:O	2.35	0.59
1:A:1978:ASN:HB3	1:A:2078:LEU:HD23	1.84	0.59
1:A:839:PRO:HB2	1:A:1614:VAL:HG11	1.83	0.58
1:A:1827:ILE:O	1:A:2059:LYS:NZ	2.37	0.58
1:A:607:ILE:HD11	1:A:785:PRO:HG2	1.87	0.57
1:A:1235:HIS:NE2	1:A:1840:ASP:OD2	2.37	0.57
1:A:1839:ASN:ND2	1:A:1840:ASP:O	2.38	0.57
1:A:1755:ILE:HG23	1:A:1756:ILE:HD12	1.87	0.56
1:A:1944:LYS:HG3	1:A:1960:PRO:HG2	1.87	0.56
1:A:655:MET:SD	1:A:655:MET:N	2.79	0.56
1:A:1946:ASP:N	1:A:1946:ASP:OD1	2.39	0.56
1:A:1959:ILE:HG23	1:A:1960:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2008:MET:SD	1:A:2016:LYS:NZ	2.75	0.56
1:A:1594:MET:HA	1:A:1597:ARG:HG3	1.87	0.56
1:A:498:ARG:NH2	1:A:538:SER:OG	2.40	0.55
1:A:1584:ASP:OD1	1:A:1620:TYR:OH	2.24	0.55
1:A:1425:GLN:HG2	1:A:1430:GLN:HA	1.89	0.54
1:A:1158:PHE:HD1	1:A:1210:TYR:HB2	1.72	0.54
1:A:1422:ARG:NH1	1:A:1442:LEU:O	2.41	0.54
1:A:1032:ARG:NH2	1:A:1041:GLU:O	2.40	0.54
1:A:828:ASN:H	1:A:831:ARG:HD2	1.72	0.53
1:A:1206:LYS:HE2	1:A:1209:LEU:HD12	1.91	0.53
1:A:1912:CYS:O	1:A:2034:ARG:NH2	2.40	0.53
1:A:1152:LYS:HA	1:A:1155:LEU:HD23	1.89	0.53
1:A:660:ARG:NH1	1:A:662:ASP:OD2	2.41	0.53
1:A:777:MET:O	2:A:2101:RTP:N3	2.41	0.53
1:A:2007:ILE:HG13	1:A:2008:MET:HG2	1.91	0.53
1:A:926:ASP:OD1	1:A:926:ASP:N	2.43	0.52
1:A:1823:HIS:HA	1:A:1826:MET:HB3	1.92	0.52
1:A:1827:ILE:HG12	1:A:2059:LYS:HZ3	1.75	0.52
1:A:584:GLU:HG2	1:A:758:LYS:HD2	1.90	0.52
1:A:1112:ILE:HD11	1:A:1217:VAL:HG23	1.92	0.52
1:A:1409:LYS:NZ	1:A:1452:ASN:O	2.42	0.52
1:A:914:LEU:HD11	1:A:1543:TYR:HB2	1.91	0.52
1:A:500:SER:O	1:A:814:ASN:ND2	2.40	0.52
1:A:1622:MET:HB3	1:A:1626:GLU:HB2	1.93	0.51
1:A:472:MET:HB2	1:A:827:LEU:HD11	1.92	0.51
1:A:485:SER:H	1:A:487:VAL:HG22	1.75	0.51
1:A:328:ARG:NH2	1:A:332:GLU:O	2.44	0.51
1:A:1205:LEU:HB3	1:A:1209:LEU:HD11	1.93	0.51
1:A:1081:MET:HG2	1:A:1389:ILE:HD12	1.93	0.51
1:A:1770:MET:SD	1:A:1851:TYR:OH	2.67	0.51
1:A:1325:ALA:HB3	1:A:1492:HIS:HB2	1.92	0.50
1:A:854:ASN:O	1:A:858:LYS:HB2	2.11	0.50
1:A:1628:ASN:OD1	1:A:1876:SER:OG	2.29	0.50
1:A:1754:GLN:NE2	1:A:1756:ILE:O	2.44	0.50
1:A:979:ASN:OD1	1:A:979:ASN:N	2.45	0.50
1:A:746:MET:HG3	1:A:1870:LEU:HD13	1.94	0.50
1:A:1110:SER:O	1:A:1110:SER:OG	2.28	0.50
1:A:873:MET:HE1	1:A:881:LEU:HD22	1.93	0.49
1:A:1195:ASN:N	1:A:1195:ASN:OD1	2.44	0.49
1:A:437:ILE:HB	1:A:921:LYS:HG2	1.94	0.49
1:A:1104:SER:HA	1:A:1223:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:TYR:O	1:A:1208:LYS:NZ	2.45	0.49
1:A:521:ASN:OD1	1:A:524:ARG:NH1	2.42	0.49
1:A:472:MET:O	1:A:825:GLN:NE2	2.44	0.49
1:A:1154:ARG:NH1	1:A:1208:LYS:O	2.45	0.49
1:A:1627:VAL:O	1:A:1632:ARG:NH2	2.45	0.49
1:A:1154:ARG:HH22	1:A:1210:TYR:H	1.59	0.48
1:A:747:VAL:HG12	1:A:758:LYS:HE2	1.93	0.48
1:A:1345:ILE:HG12	1:A:1488:ARG:HD2	1.95	0.48
1:A:397:ASP:OD1	1:A:398:LEU:N	2.47	0.48
1:A:1834:LEU:HG	1:A:2067:PHE:CD1	2.49	0.48
1:A:1845:LEU:HA	1:A:1848:LEU:HB2	1.95	0.48
1:A:711:VAL:HB	1:A:1945:ARG:HH21	1.79	0.48
1:A:1232:LYS:NZ	1:A:1238:MET:O	2.46	0.48
1:A:1391:THR:HB	1:A:1394:GLU:HG3	1.94	0.48
1:A:1819:MET:HB3	1:A:2006:LEU:HD11	1.94	0.48
1:A:1089:GLU:HG3	1:A:1312:HIS:HB3	1.94	0.48
1:A:1189:THR:OG1	1:A:1190:SER:N	2.45	0.47
1:A:1676:ASN:OD1	1:A:1679:ARG:NH2	2.47	0.47
1:A:352:THR:OG1	1:A:353:LYS:N	2.47	0.47
1:A:586:CYS:SG	1:A:587:MET:N	2.87	0.47
1:A:767:MET:HE3	1:A:790:HIS:HE1	1.78	0.47
1:A:1569:LEU:HD13	1:A:1595:LEU:HD21	1.97	0.47
1:A:447:ASN:ND2	1:A:924:ILE:O	2.43	0.47
1:A:472:MET:HE2	1:A:473:THR:H	1.79	0.47
1:A:2030:ASN:HD21	1:A:2034:ARG:HB3	1.81	0.46
1:A:1870:LEU:HA	1:A:1873:VAL:HG12	1.96	0.46
1:A:551:ASP:N	1:A:551:ASP:OD1	2.49	0.46
1:A:1622:MET:HG2	1:A:1628:ASN:HB2	1.98	0.46
1:A:1867:LYS:NZ	1:A:1871:ASP:OD2	2.46	0.46
1:A:2027:SER:OG	1:A:2032:CYS:SG	2.74	0.46
1:A:906:MET:HE2	1:A:999:VAL:HG13	1.97	0.46
1:A:427:ILE:HD11	1:A:1525:SER:HA	1.97	0.45
1:A:541:THR:HB	1:A:544:MET:HG2	1.98	0.45
1:A:495:ASN:HA	1:A:498:ARG:HB3	1.98	0.45
1:A:2058:ARG:HB3	1:A:2062:PRO:HD2	1.98	0.45
1:A:1086:GLU:HA	1:A:1091:PHE:HB2	1.99	0.44
1:A:1267:MET:HE3	1:A:1267:MET:HB3	1.89	0.44
1:A:1916:THR:OG1	1:A:2034:ARG:NH2	2.50	0.44
1:A:1266:VAL:HG21	1:A:1305:MET:HE1	1.98	0.44
1:A:1936:SER:O	1:A:1936:SER:OG	2.28	0.44
1:A:831:ARG:NH1	1:A:895:THR:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:SER:HB2	1:A:791:ILE:HB	2.00	0.44
1:A:1458:LEU:O	1:A:1462:SER:OG	2.28	0.44
1:A:2037:LYS:HA	1:A:2037:LYS:HD2	1.75	0.44
1:A:437:ILE:HD12	1:A:921:LYS:HB3	2.00	0.44
1:A:1021:LEU:HD13	1:A:1413:ILE:HG23	2.00	0.43
1:A:1345:ILE:HG23	1:A:1501:ILE:HD11	2.00	0.43
1:A:1081:MET:HE1	1:A:1320:SER:HB2	1.99	0.43
1:A:1726:LEU:HD23	1:A:1726:LEU:HA	1.89	0.43
1:A:1782:ASN:OD1	1:A:1782:ASN:N	2.52	0.43
1:A:2058:ARG:HD2	1:A:2061:PHE:H	1.83	0.43
1:A:1735:VAL:HA	1:A:1753:THR:HB	2.00	0.43
1:A:1786:ASN:HA	1:A:1787:GLU:HA	1.81	0.43
1:A:1509:MET:HA	1:A:1512:ASP:HB2	2.00	0.43
1:A:1831:GLU:HB2	1:A:1835:ILE:HD11	2.00	0.43
1:A:1145:ILE:HD11	1:A:1176:ILE:HG22	2.01	0.42
1:A:491:ASN:HD22	1:A:491:ASN:C	2.26	0.42
1:A:1357:LYS:HB2	1:A:1357:LYS:HE3	1.79	0.42
1:A:1586:MET:HE3	1:A:1648:THR:HG21	2.00	0.42
1:A:1920:LEU:HD13	1:A:1986:LYS:HB3	2.00	0.42
1:A:1701:GLN:HG2	1:A:1911:TYR:CZ	2.55	0.42
1:A:1096:TYR:OH	1:A:1840:ASP:OD1	2.36	0.42
1:A:775:ASP:OD1	1:A:775:ASP:N	2.47	0.42
1:A:1841:ARG:H	1:A:1844:LEU:HD12	1.83	0.42
1:A:1879:ARG:HG2	1:A:1891:THR:HG23	2.01	0.42
1:A:1956:GLU:HG3	1:A:1957:LYS:HE2	2.01	0.42
1:A:471:SER:OG	1:A:472:MET:SD	2.70	0.42
1:A:1120:GLU:O	1:A:1124:ASN:ND2	2.53	0.42
1:A:1631:ILE:H	1:A:1631:ILE:HG12	1.68	0.42
1:A:439:ASP:OD1	1:A:439:ASP:N	2.52	0.42
1:A:1028:GLU:OE2	1:A:1032:ARG:NH1	2.45	0.42
1:A:1747:LYS:HD3	1:A:1747:LYS:HA	1.75	0.41
1:A:333:ILE:H	1:A:336:SER:HB3	1.84	0.41
1:A:544:MET:HE3	1:A:572:ASN:HD22	1.85	0.41
1:A:1490:ILE:HB	1:A:1497:ALA:HB3	2.02	0.41
1:A:1605:ILE:HD13	1:A:1605:ILE:HA	1.91	0.41
1:A:1641:LEU:HD23	1:A:1722:LYS:HG2	2.02	0.41
1:A:680:LEU:HD21	1:A:800:PHE:HD1	1.86	0.41
1:A:997:ASN:HA	1:A:1566:CYS:SG	2.60	0.41
1:A:370:THR:HG21	1:A:1077:ASN:HA	2.02	0.41
1:A:1107:CYS:N	1:A:1221:LYS:O	2.54	0.41
1:A:1590:ILE:O	1:A:1594:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1986:LYS:C	1:A:1989:PRO:HD2	2.46	0.41
1:A:937:ASP:OD1	1:A:937:ASP:N	2.51	0.41
1:A:1193:ILE:HD12	1:A:1201:VAL:HG13	2.03	0.41
1:A:1271:LYS:HE2	1:A:1271:LYS:HB3	1.74	0.41
1:A:1413:ILE:H	1:A:1413:ILE:HG13	1.61	0.41
1:A:1853:SER:HB3	1:A:1856:LYS:HB2	2.02	0.41
1:A:1562:ILE:HA	1:A:1563:PRO:HD3	1.96	0.41
1:A:600:LYS:HB2	1:A:600:LYS:HE3	1.71	0.40
1:A:1390:LEU:HD23	1:A:1390:LEU:HA	1.80	0.40
1:A:567:LYS:HB3	1:A:568:SER:H	1.78	0.40
1:A:995:LEU:O	1:A:999:VAL:HG23	2.21	0.40
1:A:1750:THR:OG1	1:A:1751:MET:N	2.54	0.40
1:A:370:THR:OG1	1:A:1078:VAL:N	2.44	0.40
1:A:1173:LEU:HA	1:A:1176:ILE:HB	2.03	0.40
1:A:595:LYS:HE3	1:A:595:LYS:HB2	1.82	0.40
1:A:666:SER:HB3	1:A:935:VAL:HG13	2.01	0.40
1:A:1716:LEU:HD23	1:A:1716:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1667/1766 (94%)	1507 (90%)	156 (9%)	4 (0%)	44 74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1959	ILE
1	A	567	LYS
1	A	1493	SER
1	A	1215	VAL

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	1535/1634 (94%)	1472 (96%)	63 (4%)	26 57

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	LYS
1	A	435	LYS
1	A	472	MET
1	A	482	GLU
1	A	483	LEU
1	A	491	ASN
1	A	495	ASN
1	A	516	ILE
1	A	534	LEU
1	A	561	LYS
1	A	562	VAL
1	A	574	GLN
1	A	655	MET
1	A	726	CYS
1	A	760	LEU
1	A	769	LEU
1	A	792	VAL
1	A	793	ASP
1	A	826	ARG
1	A	840	SER
1	A	874	THR
1	A	894	VAL
1	A	914	LEU
1	A	1012	ASN
1	A	1013	HIS
1	A	1020	LEU
1	A	1029	LEU
1	A	1058	ILE
1	A	1110	SER
1	A	1155	LEU

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Mol	Chain	Res	Type
1	A	1167	LEU
1	A	1170	VAL
1	A	1188	VAL
1	A	1195	ASN
1	A	1209	LEU
1	A	1217	VAL
1	A	1260	LEU
1	A	1342	LEU
1	A	1359	SER
1	A	1402	ILE
1	A	1483	CYS
1	A	1518	LEU
1	A	1574	THR
1	A	1620	TYR
1	A	1630	SER
1	A	1712	GLU
1	A	1715	THR
1	A	1743	THR
1	A	1769	LYS
1	A	1795	LYS
1	A	1925	VAL
1	A	1929	MET
1	A	1938	TYR
1	A	1946	ASP
1	A	1956	GLU
1	A	1958	TRP
1	A	1959	ILE
1	A	1994	SER
1	A	2002	PHE
1	A	2015	VAL
1	A	2021	PHE
1	A	2055	CYS
1	A	2080	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
1	A	372	ASN
1	A	384	GLN
1	A	461	ASN
1	A	581	ASN

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Mol	Chain	Res	Type
1	A	663	ASN
1	A	879	GLN
1	A	998	ASN
1	A	1074	ASN
1	A	1319	GLN
1	A	1368	GLN
1	A	1431	ASN
1	A	1486	GLN
1	A	1628	ASN
1	A	1754	GLN
1	A	1839	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](#)

2 ligands are modelled in this entry.

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
2	RTP	A	2102	-	23,30,30	3.39	8 (34%)	29,47,47	2.02	5 (17%)
2	RTP	A	2101	-	23,30,30	3.38	8 (34%)	29,47,47	2.00	4 (13%)

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
2	RTP	A	2102	-	-	6/18/42/42	0/2/2/2
2	RTP	A	2101	-	-	7/18/42/42	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2102	RTP	C3'-C4'	-8.73	1.30	1.53
2	A	2101	RTP	C3'-C4'	-8.64	1.30	1.53
2	A	2101	RTP	O4'-C4'	8.42	1.63	1.45
2	A	2102	RTP	O4'-C4'	8.26	1.63	1.45
2	A	2102	RTP	O4'-C1'	-7.55	1.30	1.41
2	A	2101	RTP	O4'-C1'	-7.39	1.30	1.41
2	A	2101	RTP	C6-N3	4.77	1.42	1.33
2	A	2102	RTP	C6-N3	4.70	1.41	1.33
2	A	2101	RTP	O3'-C3'	3.22	1.50	1.43
2	A	2102	RTP	O3'-C3'	3.19	1.50	1.43
2	A	2102	RTP	PA-O5'	2.86	1.70	1.59
2	A	2101	RTP	PA-O5'	2.85	1.70	1.59
2	A	2101	RTP	O2'-C2'	-2.56	1.36	1.43
2	A	2102	RTP	O2'-C2'	-2.54	1.37	1.43
2	A	2102	RTP	C3-N2	-2.43	1.31	1.34
2	A	2101	RTP	C3-N2	-2.20	1.32	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2101	RTP	N2-C3-N4	-8.78	107.44	114.72
2	A	2102	RTP	N2-C3-N4	-8.61	107.58	114.72
2	A	2102	RTP	PB-O3B-PG	-2.76	123.37	132.83
2	A	2102	RTP	PA-O3A-PB	-2.62	123.82	132.83
2	A	2101	RTP	PB-O3B-PG	-2.55	124.07	132.83
2	A	2102	RTP	C3'-C2'-C1'	2.55	104.82	100.98
2	A	2101	RTP	C3-C6-N3	2.45	119.94	115.85
2	A	2102	RTP	C2'-C3'-C4'	2.10	106.73	102.64
2	A	2101	RTP	O4'-C1'-C2'	-2.01	103.99	106.93

There are no chirality outliers.

All (13) torsion outliers are listed below:

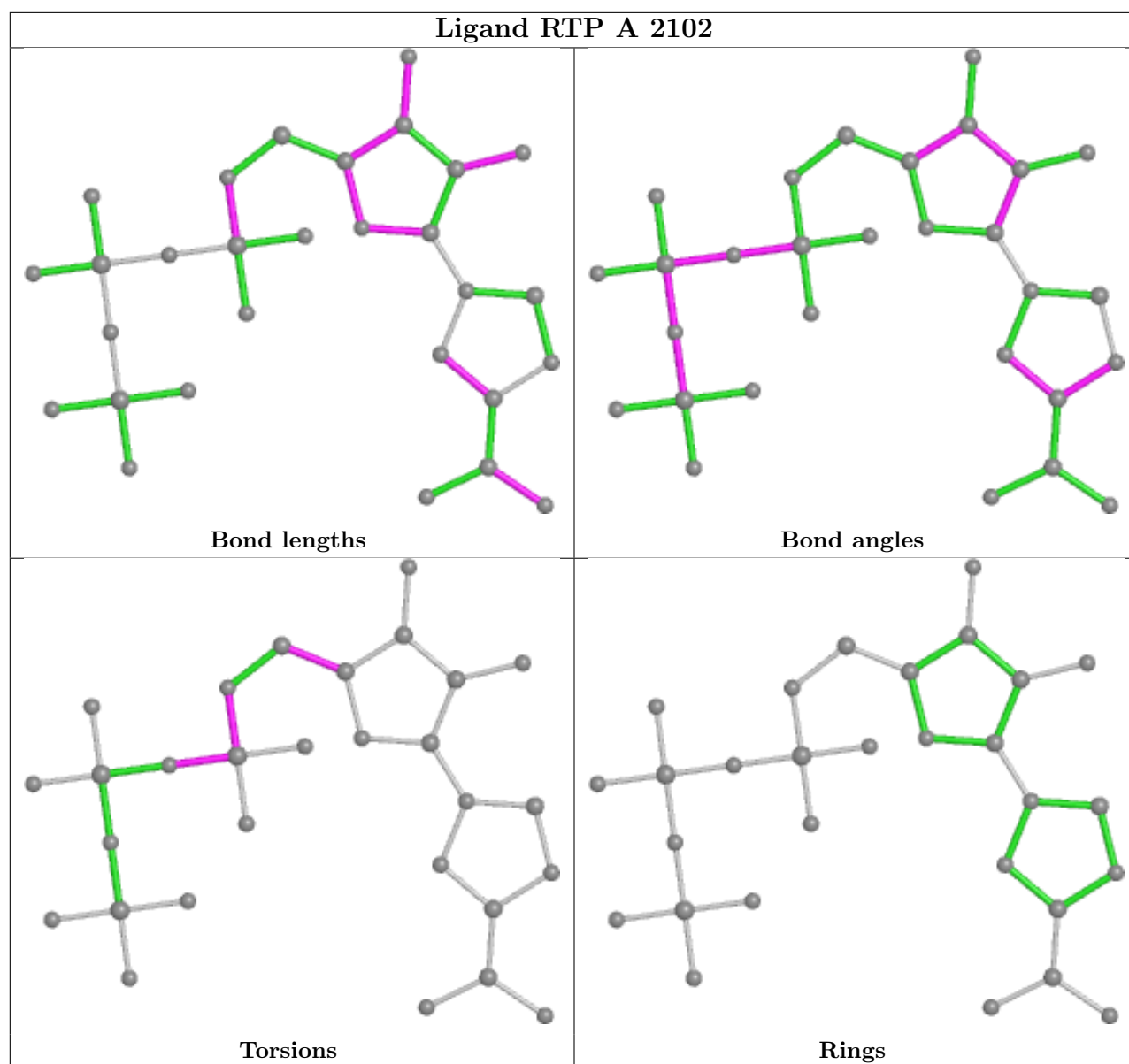
Mol	Chain	Res	Type	Atoms
2	A	2101	RTP	C5'-O5'-PA-O3A
2	A	2101	RTP	C5'-O5'-PA-O1A
2	A	2101	RTP	C5'-O5'-PA-O2A
2	A	2102	RTP	C5'-O5'-PA-O3A
2	A	2102	RTP	O4'-C4'-C5'-O5'
2	A	2102	RTP	C3'-C4'-C5'-O5'
2	A	2101	RTP	O4'-C4'-C5'-O5'
2	A	2102	RTP	C5'-O5'-PA-O1A
2	A	2101	RTP	C3'-C4'-C5'-O5'
2	A	2102	RTP	PB-O3A-PA-O1A
2	A	2101	RTP	C4'-C5'-O5'-PA
2	A	2102	RTP	PB-O3A-PA-O5'
2	A	2101	RTP	PG-O3B-PB-O2B

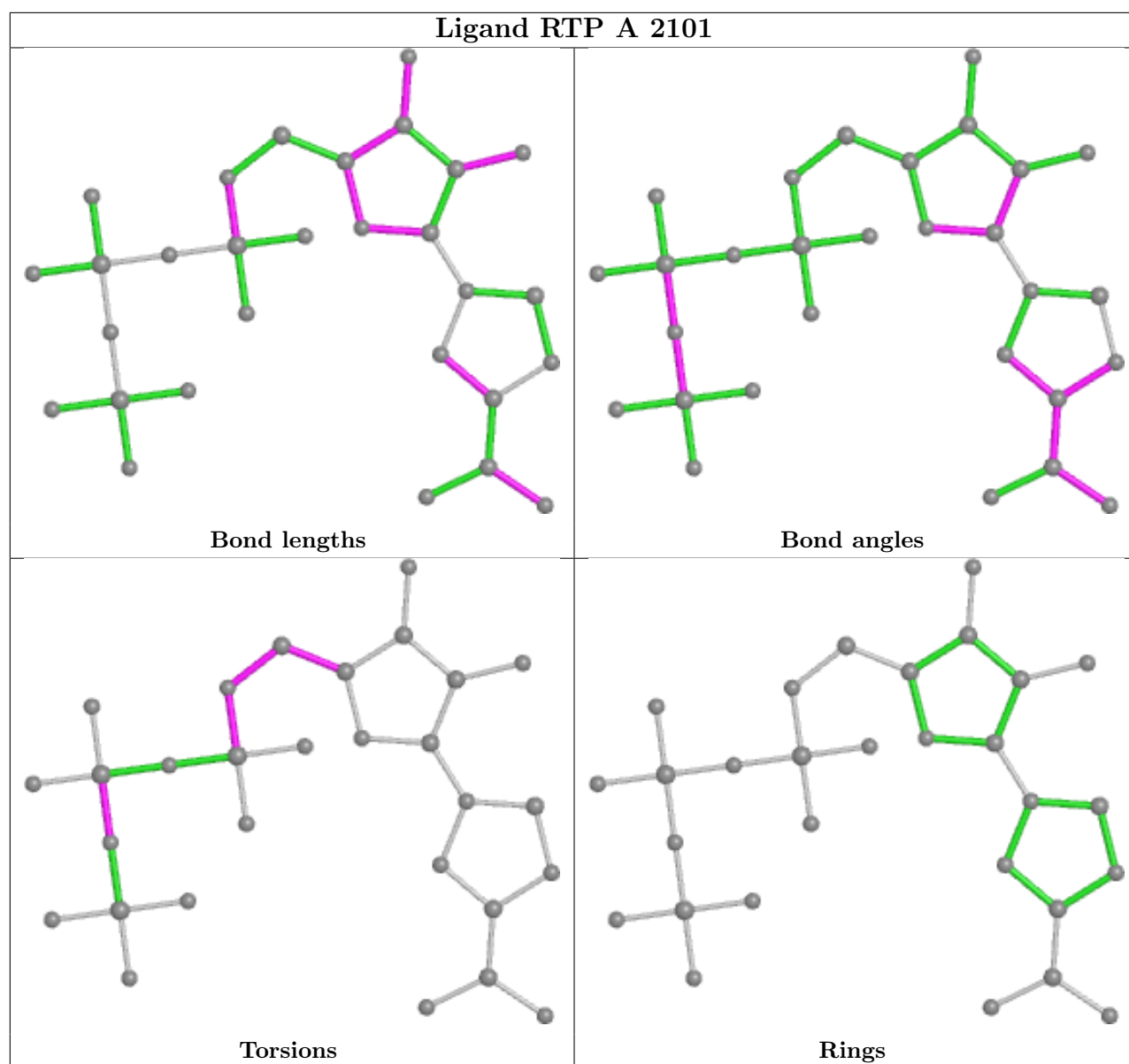
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2102	RTP	1	0
2	A	2101	RTP	2	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.