WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Feb 20, 2025 – 12:06 pm GMT

|		
PDB ID	:	9F2W
EMDB ID	:	EMD-50165
Title	:	Cryo-EM structure of the I923V MDA5-dsRNA filament in complex with ATP
Authors	:	Singh, R.; Herrero del Valle, A.; Modis, Y.
Deposited on	:	2024-04-24
Resolution	:	4.21 Å(reported)
Based on initial model	:	7BKQ
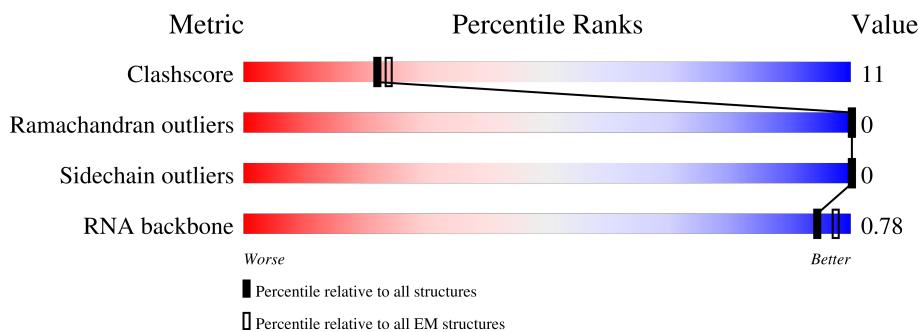
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
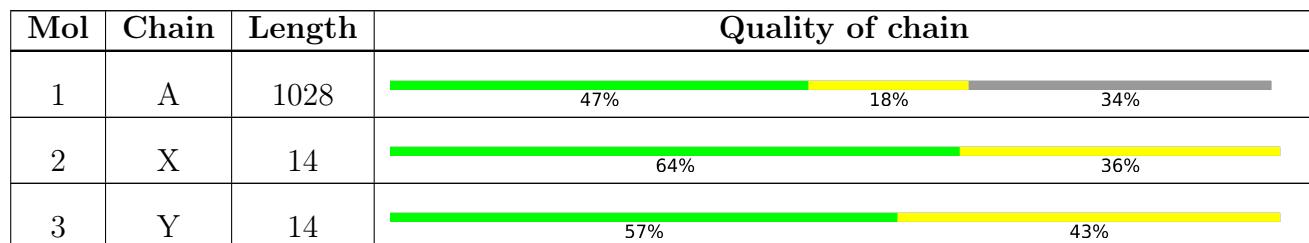
The reported resolution of this entry is 4.21 Å.

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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		0
RNA backbone		0.78

Worse　　　　　*Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1028	47% 18% 34%
2	X	14	64% 36%
3	Y	14	57% 43%

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2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11718 atoms, of which 5737 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 Interferon-induced helicase C domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	675	10774	3393	5421	935	992	33	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q8R5F7
A	-19	GLY	-	expression tag	UNP Q8R5F7
A	-18	SER	-	expression tag	UNP Q8R5F7
A	-17	SER	-	expression tag	UNP Q8R5F7
A	-16	HIS	-	expression tag	UNP Q8R5F7
A	-15	HIS	-	expression tag	UNP Q8R5F7
A	-14	HIS	-	expression tag	UNP Q8R5F7
A	-13	HIS	-	expression tag	UNP Q8R5F7
A	-12	HIS	-	expression tag	UNP Q8R5F7
A	-11	HIS	-	expression tag	UNP Q8R5F7
A	-10	SER	-	expression tag	UNP Q8R5F7
A	-9	SER	-	expression tag	UNP Q8R5F7
A	-8	GLY	-	expression tag	UNP Q8R5F7
A	-7	ARG	-	expression tag	UNP Q8R5F7
A	-6	GLU	-	expression tag	UNP Q8R5F7
A	-5	ASN	-	expression tag	UNP Q8R5F7
A	-4	LEU	-	expression tag	UNP Q8R5F7
A	-3	TYR	-	expression tag	UNP Q8R5F7
A	-2	PHE	-	expression tag	UNP Q8R5F7
A	-1	GLN	-	expression tag	UNP Q8R5F7
A	0	GLY	-	expression tag	UNP Q8R5F7
A	1	HIS	-	expression tag	UNP Q8R5F7
A	2	MET	-	expression tag	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	LYS	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q8R5F7
A	?	-	ALA	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	CYS	deletion	UNP Q8R5F7
A	?	-	ASN	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	GLN	deletion	UNP Q8R5F7
A	?	-	LEU	deletion	UNP Q8R5F7
A	?	-	LYS	deletion	UNP Q8R5F7
A	?	-	GLY	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	VAL	deletion	UNP Q8R5F7
A	923	VAL	ILE	engineered mutation	UNP Q8R5F7

- Molecule 2 is a RNA chain called RNA (5'-R(P*CP*AP*AP*GP*CP*CP*GP*AP*GP*GP *AP*GP*AP*U)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	X	14	459	136	154	61	94	14	0	0
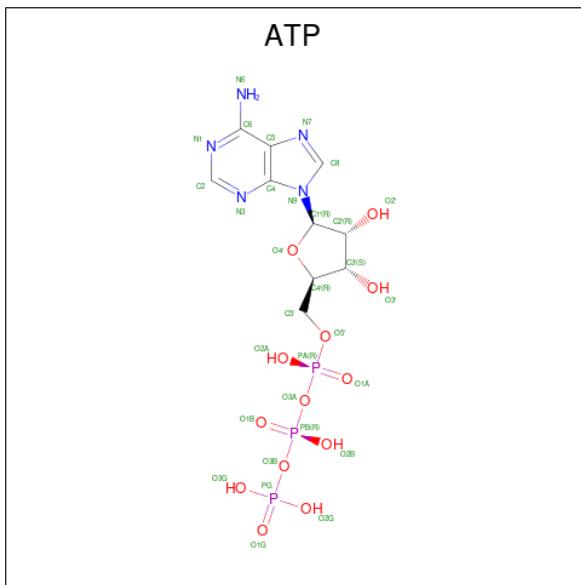
- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*UP*CP*UP*CP*CP*UP*CP*GP*GP *CP*UP*UP*G)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
3	Y	14	441	130	150	45	102	14	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

ATP
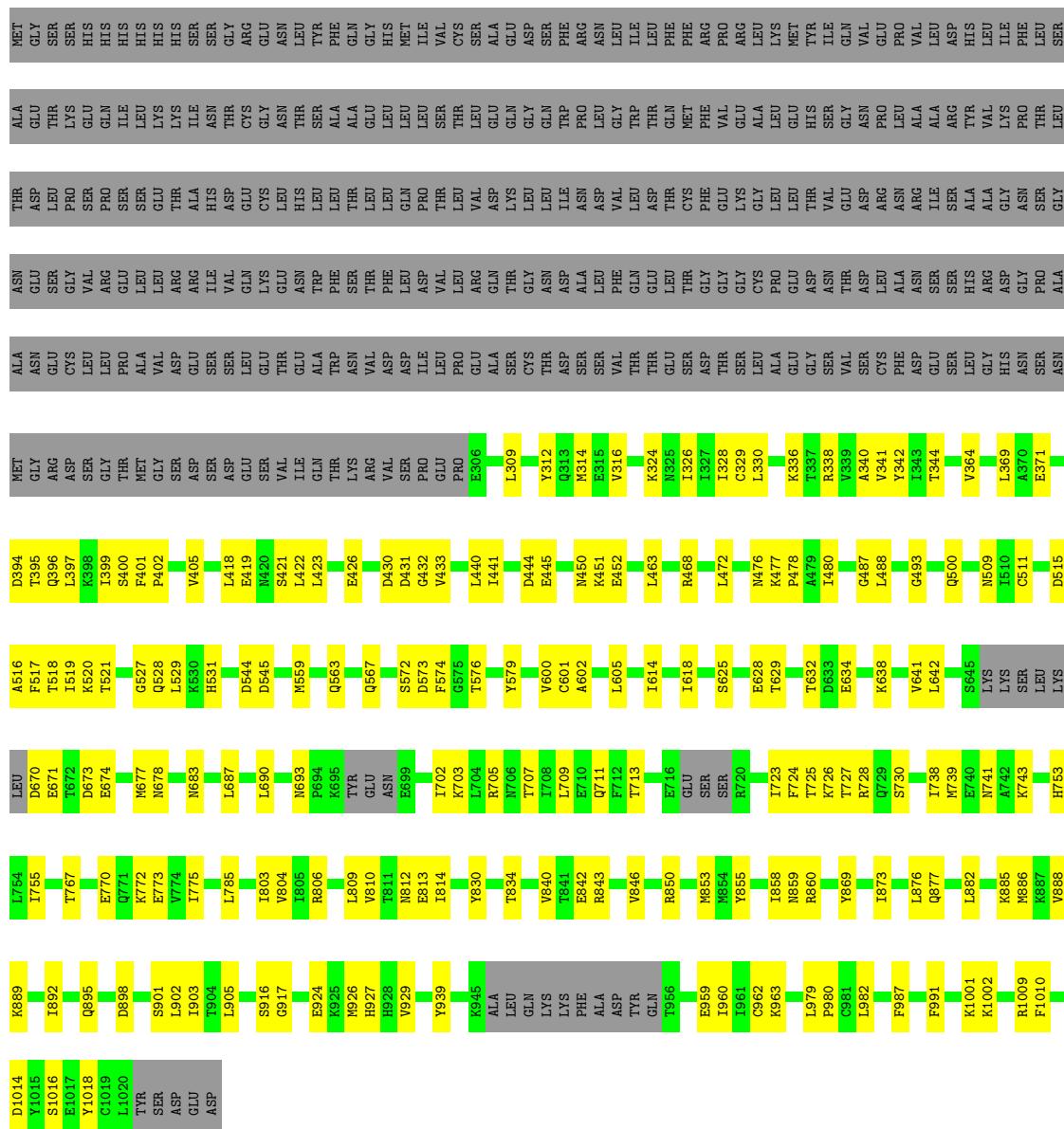
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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: Interferon-induced helicase C domain-containing protein 1
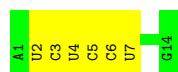
• Molecule 2: RNA (5'-R(P*CP*AP*AP*GP*CP*CP*GP*AP*GP*GP*AP*GP*AP*U)-3')

Chain X:

• Molecule 3: RNA (5'-R(P*AP*UP*CP*UP*CP*CP*UP*CP*GP*GP*CP*UP*UP*G)-3')

Chain Y:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=84.15°, rise=43.92 Å, axial sym=C1	Depositor
Number of segments used	337327	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k 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: ZN, ATP

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	0.27	0/5438	0.48	0/7320
2	X	0.35	0/342	0.75	0/532
3	Y	0.35	0/322	0.80	0/498
All	All	0.28	0/6102	0.52	0/8350

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 ⓘ

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	5353	5421	5421	128	0
2	X	305	154	154	4	0
3	Y	291	150	150	7	0
4	A	1	0	0	0	0
5	A	31	12	12	1	0
All	All	5981	5737	5737	132	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 (132) 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:1002:LYS:NZ	2:X:6:C:OP1	1.97	0.96
1:A:727:THR:O	1:A:730:SER:OG	1.91	0.88
1:A:842:GLU:O	1:A:846:VAL:HG23	1.77	0.85
1:A:371:GLU:OE2	1:A:772:LYS:NZ	2.12	0.81
1:A:614:ILE:O	1:A:618:ILE:N	2.17	0.76
1:A:430:ASP:OD1	1:A:431:ASP:N	2.21	0.74
1:A:927:HIS:NE2	2:X:4:G:O2'	2.21	0.74
1:A:703:LYS:O	1:A:707:THR:HG23	1.88	0.73
1:A:431:ASP:OD1	1:A:432:GLY:N	2.21	0.73
1:A:399:ILE:O	1:A:400:SER:OG	2.08	0.71
1:A:671:GLU:N	1:A:671:GLU:OE1	2.24	0.71
1:A:472:LEU:O	1:A:476:ASN:N	2.23	0.70
1:A:901:SER:O	1:A:902:LEU:HD23	1.92	0.69
1:A:705:ARG:HH11	1:A:709:LEU:HD12	1.58	0.69
1:A:905:LEU:HD21	1:A:987:PHE:CD2	2.28	0.68
1:A:394:ASP:OD1	1:A:395:THR:N	2.27	0.68
1:A:625:SER:O	1:A:629:THR:HG23	1.94	0.68
1:A:728:ARG:HD3	1:A:755:ILE:HD12	1.74	0.68
1:A:527:GLY:O	1:A:531:HIS:ND1	2.27	0.68
1:A:709:LEU:O	1:A:713:THR:HG23	1.93	0.67
1:A:519:ILE:HG21	1:A:858:ILE:HD11	1.78	0.66
1:A:959:GLU:N	1:A:959:GLU:OE1	2.29	0.66
1:A:929:VAL:HG21	1:A:979:LEU:HD22	1.76	0.66
1:A:444:ASP:OD1	1:A:445:GLU:N	2.30	0.65
1:A:329:CYS:SG	1:A:521:THR:OG1	2.52	0.65
1:A:929:VAL:HG23	1:A:980:PRO:O	1.97	0.64
1:A:869:TYR:O	1:A:873:ILE:HD12	1.98	0.63
1:A:1001:LYS:NZ	3:Y:4:U:OP1	2.29	0.61
1:A:889:LYS:O	1:A:892:ILE:HG22	2.01	0.61
1:A:813:GLU:OE1	1:A:850:ARG:NH1	2.34	0.61
1:A:1014:ASP:OD2	1:A:1016:SER:OG	2.20	0.59
1:A:450:ASN:ND2	2:X:10:G:OP1	2.35	0.59
1:A:642:LEU:HD23	1:A:642:LEU:O	2.03	0.59
1:A:728:ARG:NE	3:Y:7:U:OP1	2.35	0.59
1:A:859:ASN:OD1	1:A:860:ARG:N	2.36	0.57
1:A:885:LYS:O	1:A:888:VAL:HG12	2.05	0.57
1:A:628:GLU:O	1:A:632:THR:HG23	2.05	0.56
1:A:962:CYS:SG	1:A:963:LYS:N	2.78	0.56
1:A:806:ARG:NH2	1:A:809:LEU:O	2.38	0.56
1:A:338:ARG:HA	1:A:341:VAL:HG22	1.88	0.56
1:A:674:GLU:O	1:A:678:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ASN:HA	1:A:876:LEU:HD13	1.87	0.56
1:A:573:ASP:OD1	1:A:574:PHE:N	2.40	0.54
1:A:511:CYS:O	1:A:515:ASP:N	2.40	0.54
1:A:690:LEU:O	1:A:693:ASN:ND2	2.41	0.54
1:A:309:LEU:HD11	1:A:342:TYR:CE1	2.43	0.53
1:A:1009:ARG:NH2	1:A:1010:PHE:O	2.41	0.53
1:A:724:PHE:HB3	1:A:809:LEU:HD23	1.91	0.53
1:A:463:LEU:HD13	1:A:877:GLN:HG2	1.92	0.52
1:A:810:VAL:HG11	1:A:843:ARG:HB2	1.90	0.52
1:A:834:THR:HG21	1:A:840:VAL:HB	1.90	0.52
1:A:1002:LYS:HZ3	2:X:6:C:P	2.25	0.52
1:A:725:THR:O	1:A:809:LEU:HD22	2.10	0.52
1:A:364:VAL:HG11	1:A:369:LEU:HB2	1.91	0.51
1:A:895:GLN:NE2	1:A:898:ASP:OD1	2.41	0.51
1:A:397:LEU:H	1:A:397:LEU:HD23	1.75	0.51
1:A:312:TYR:CG	1:A:529:LEU:HD21	2.47	0.50
1:A:869:TYR:CE1	1:A:873:ILE:HD11	2.47	0.50
1:A:528:GLN:OE1	1:A:528:GLN:N	2.44	0.50
1:A:772:LYS:O	1:A:775:ILE:HG22	2.12	0.49
1:A:982:LEU:HD23	1:A:982:LEU:H	1.76	0.49
1:A:810:VAL:HG13	1:A:810:VAL:O	2.12	0.49
1:A:452:GLU:O	1:A:452:GLU:HG3	2.12	0.49
1:A:421:SER:OG	1:A:433:VAL:HG12	2.13	0.49
1:A:855:TYR:HA	1:A:858:ILE:HG22	1.94	0.49
1:A:882:LEU:O	1:A:886:MET:HG2	2.13	0.48
1:A:924:GLU:O	1:A:926:MET:HG2	2.13	0.48
1:A:602:ALA:HA	1:A:605:LEU:HD12	1.96	0.48
1:A:396:GLN:N	1:A:396:GLN:OE1	2.46	0.48
1:A:309:LEU:HD11	1:A:342:TYR:CD1	2.48	0.48
1:A:487:GLY:C	1:A:488:LEU:HD22	2.34	0.48
1:A:316:VAL:HG21	1:A:328:ILE:HG23	1.96	0.48
1:A:711:GLN:NE2	1:A:803:ILE:HD11	2.29	0.47
1:A:440:LEU:HD12	1:A:441:ILE:N	2.29	0.47
1:A:576:THR:HG23	1:A:579:TYR:H	1.79	0.47
1:A:340:ALA:O	1:A:344:THR:HG23	2.14	0.47
1:A:511:CYS:SG	1:A:519:ILE:HD11	2.55	0.47
1:A:517:PHE:O	1:A:518:THR:HG23	2.14	0.47
1:A:723:ILE:HD13	1:A:785:LEU:HD21	1.96	0.46
1:A:563:GLN:O	1:A:567:GLN:N	2.49	0.46
1:A:493:GLY:CA	1:A:814:ILE:HD11	2.45	0.46
1:A:705:ARG:NH1	1:A:709:LEU:HD12	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:SER:C	1:A:902:LEU:HD23	2.37	0.46
1:A:559:MET:CE	1:A:605:LEU:HD22	2.45	0.45
1:A:418:LEU:O	1:A:422:LEU:HG	2.17	0.45
1:A:468:ARG:O	1:A:472:LEU:HD13	2.17	0.45
1:A:702:ILE:HG13	1:A:703:LYS:N	2.32	0.45
1:A:741:ASN:OD1	1:A:743:LYS:N	2.47	0.45
1:A:572:SER:OG	1:A:573:ASP:N	2.50	0.44
1:A:336:LYS:NZ	5:A:1102:ATP:O1B	2.42	0.44
1:A:450:ASN:CG	1:A:451:LYS:H	2.21	0.44
1:A:477:LYS:N	1:A:478:PRO:HD2	2.32	0.44
1:A:674:GLU:HA	1:A:677:MET:HG2	2.00	0.43
3:Y:2:U:H2'	3:Y:3:C:C6	2.54	0.43
1:A:468:ARG:CZ	1:A:468:ARG:HA	2.49	0.43
1:A:516:ALA:O	1:A:517:PHE:HB2	2.19	0.43
1:A:309:LEU:HB3	1:A:314:MET:HE2	2.00	0.43
1:A:401:PHE:N	1:A:402:PRO:CD	2.82	0.43
1:A:753:HIS:O	1:A:753:HIS:ND1	2.51	0.43
1:A:812:ASN:OD1	1:A:813:GLU:N	2.51	0.43
1:A:500:GLN:HA	1:A:853:MET:HE3	2.01	0.42
1:A:939:TYR:CD1	1:A:960:ILE:HG23	2.55	0.42
1:A:329:CYS:O	1:A:330:LEU:HD23	2.20	0.42
1:A:426:GLU:HA	1:A:426:GLU:OE1	2.19	0.42
1:A:767:THR:OG1	1:A:770:GLU:HB2	2.20	0.42
1:A:1018:TYR:O	1:A:1018:TYR:CG	2.72	0.42
1:A:520:LYS:HE3	1:A:520:LYS:HA	2.02	0.42
3:Y:3:C:H2'	3:Y:4:U:H6	1.84	0.42
1:A:324:LYS:O	1:A:326:ILE:HG23	2.19	0.42
1:A:634:GLU:O	1:A:638:LYS:HG2	2.20	0.42
1:A:903:ILE:HG22	1:A:991:PHE:CD1	2.55	0.42
1:A:683:ASN:O	1:A:687:LEU:HG	2.20	0.41
1:A:419:GLU:O	1:A:423:LEU:HG	2.21	0.41
1:A:670:ASP:O	1:A:673:ASP:N	2.51	0.41
1:A:480:ILE:H	1:A:480:ILE:HD12	1.85	0.41
1:A:517:PHE:O	1:A:518:THR:CG2	2.68	0.41
1:A:518:THR:O	1:A:519:ILE:HD13	2.21	0.41
1:A:559:MET:HE1	1:A:605:LEU:HD22	2.02	0.41
3:Y:4:U:H2'	3:Y:5:C:H6	1.85	0.41
1:A:813:GLU:HG2	1:A:814:ILE:N	2.35	0.41
1:A:544:ASP:OD1	1:A:545:ASP:N	2.54	0.41
1:A:600:VAL:HG13	1:A:601:CYS:N	2.36	0.41
1:A:638:LYS:HA	1:A:641:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:PHE:O	1:A:405:VAL:HG23	2.21	0.40
1:A:726:LYS:NZ	3:Y:6:C:O4'	2.40	0.40
1:A:738:ILE:HG23	1:A:739:MET:HE2	2.03	0.40
1:A:493:GLY:HA2	1:A:814:ILE:HD11	2.03	0.40
3:Y:2:U:H2'	3:Y:3:C:H6	1.86	0.40
1:A:709:LEU:CD1	1:A:743:LYS:HE3	2.51	0.40
1:A:804:VAL:O	1:A:830:TYR:HA	2.22	0.40
1:A:770:GLU:HA	1:A:773:GLU:CD	2.42	0.40
1:A:916:SER:OG	1:A:917:GLY:N	2.54	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	665/1028 (65%)	624 (94%)	41 (6%)	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	586/918 (64%)	586 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	711	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	13/14 (92%)	2 (15%)	0
3	Y	13/14 (92%)	0	0
All	All	26/28 (92%)	2 (7%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	13	A
2	X	14	U

There are no RNA pucker outliers to report.

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	$\#\|Z\| > 2$
5	ATP	A	1102	-	26,33,33	0.61	0	31,52,52	1.10	2 (6%)

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
5	ATP	A	1102	-	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1102	ATP	C5-C6-N6	2.17	123.65	120.35
5	A	1102	ATP	PB-O3B-PG	2.04	139.83	132.83

There are no chirality outliers.
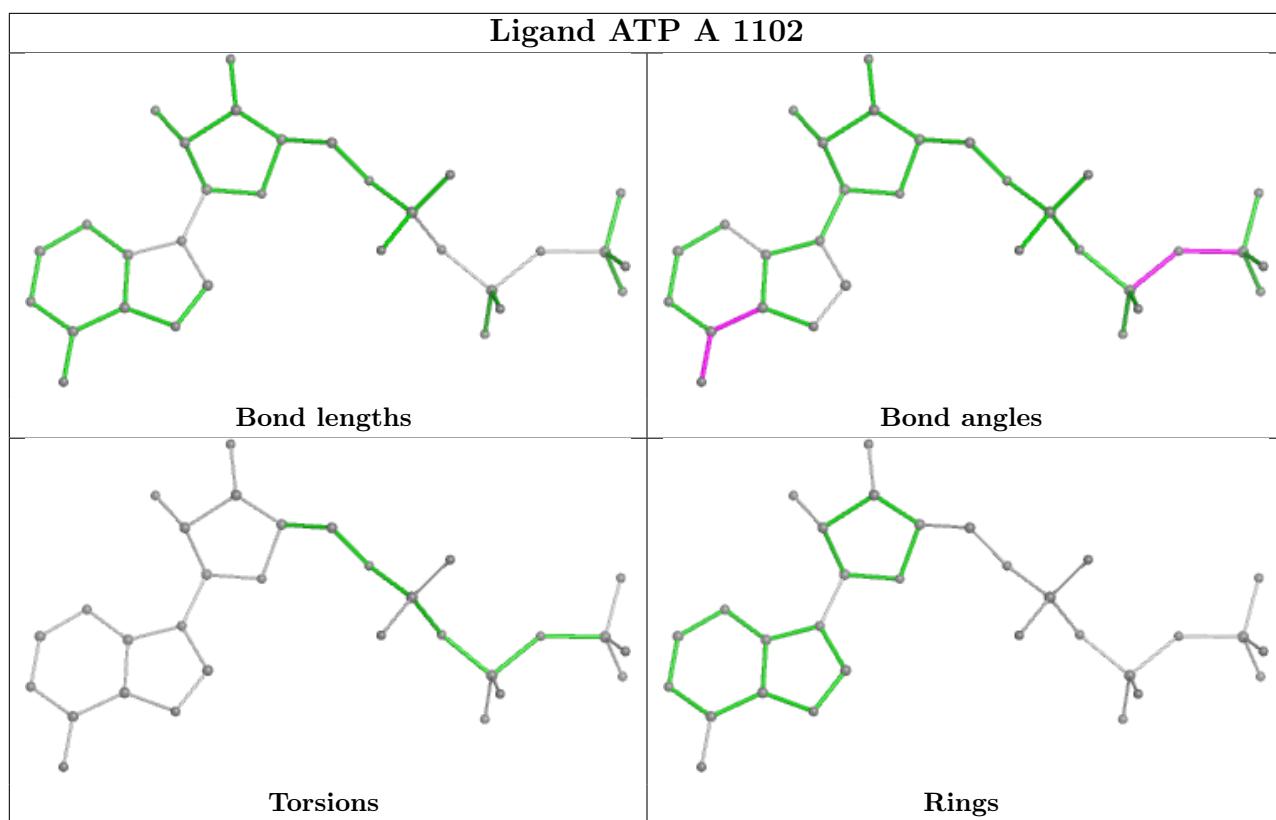
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1102	ATP	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 then 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.

Ligand ATP A 1102

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.