



Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 02:12 PM JST

PDB ID : 9J3N / pdb_00009j3n
EMDB ID : EMD-61120
Title : ATP bound Chlamydia pneumoniae ATP/ADP translocator NTT1(Inward open state)
Authors : Lin, H.J.; Huang, J.; Li, T.M.; Li, W.J.; Su, N.N.; Zhang, J.R.; Wu, X.D.; Fan, M.R.
Deposited on : 2024-08-08
Resolution : 2.72 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

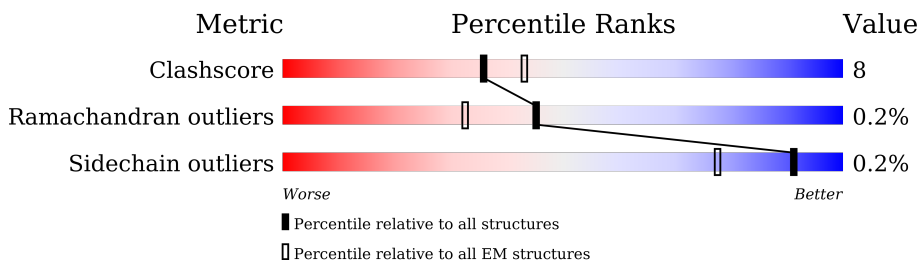
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.72 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	B	121	
2	A	586	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4809 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 1D10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	121	Total	C	N	O	S	0	0
			949	596	164	185	4		

- Molecule 2 is a protein called ADP,ATP carrier protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	488	Total	C	N	O	S	0	0
			3829	2565	607	634	23		

There are 71 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	VAL	-	expression tag	UNP Q9Z8J2
A	517	ASP	-	expression tag	UNP Q9Z8J2
A	518	GLU	-	expression tag	UNP Q9Z8J2
A	519	LEU	-	expression tag	UNP Q9Z8J2
A	520	THR	-	expression tag	UNP Q9Z8J2
A	521	SER	-	expression tag	UNP Q9Z8J2
A	522	ARG	-	expression tag	UNP Q9Z8J2
A	523	GLY	-	expression tag	UNP Q9Z8J2
A	524	ARG	-	expression tag	UNP Q9Z8J2
A	525	GLY	-	expression tag	UNP Q9Z8J2
A	526	SER	-	expression tag	UNP Q9Z8J2
A	527	GLY	-	expression tag	UNP Q9Z8J2
A	528	GLY	-	expression tag	UNP Q9Z8J2
A	529	LEU	-	expression tag	UNP Q9Z8J2
A	530	ASN	-	expression tag	UNP Q9Z8J2
A	531	ASP	-	expression tag	UNP Q9Z8J2
A	532	ILE	-	expression tag	UNP Q9Z8J2
A	533	PHE	-	expression tag	UNP Q9Z8J2
A	534	GLU	-	expression tag	UNP Q9Z8J2
A	535	ALA	-	expression tag	UNP Q9Z8J2
A	536	GLN	-	expression tag	UNP Q9Z8J2

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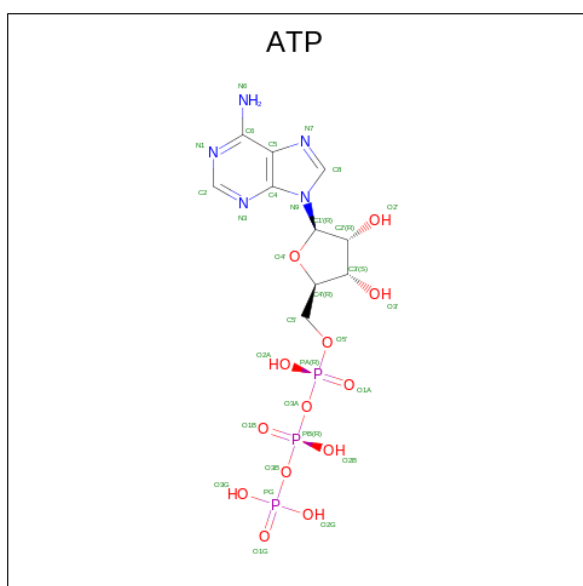
Chain	Residue	Modelled	Actual	Comment	Reference
A	537	LYS	-	expression tag	UNP Q9Z8J2
A	538	ILE	-	expression tag	UNP Q9Z8J2
A	539	GLU	-	expression tag	UNP Q9Z8J2
A	540	TRP	-	expression tag	UNP Q9Z8J2
A	541	HIS	-	expression tag	UNP Q9Z8J2
A	542	GLU	-	expression tag	UNP Q9Z8J2
A	543	GLY	-	expression tag	UNP Q9Z8J2
A	544	SER	-	expression tag	UNP Q9Z8J2
A	545	GLY	-	expression tag	UNP Q9Z8J2
A	546	LEU	-	expression tag	UNP Q9Z8J2
A	547	GLU	-	expression tag	UNP Q9Z8J2
A	548	VAL	-	expression tag	UNP Q9Z8J2
A	549	LEU	-	expression tag	UNP Q9Z8J2
A	550	PHE	-	expression tag	UNP Q9Z8J2
A	551	GLN	-	expression tag	UNP Q9Z8J2
A	552	GLY	-	expression tag	UNP Q9Z8J2
A	553	PRO	-	expression tag	UNP Q9Z8J2
A	554	ASP	-	expression tag	UNP Q9Z8J2
A	555	TYR	-	expression tag	UNP Q9Z8J2
A	556	LYS	-	expression tag	UNP Q9Z8J2
A	557	ASP	-	expression tag	UNP Q9Z8J2
A	558	ASP	-	expression tag	UNP Q9Z8J2
A	559	ASP	-	expression tag	UNP Q9Z8J2
A	560	ASP	-	expression tag	UNP Q9Z8J2
A	561	LYS	-	expression tag	UNP Q9Z8J2
A	562	TRP	-	expression tag	UNP Q9Z8J2
A	563	SER	-	expression tag	UNP Q9Z8J2
A	564	HIS	-	expression tag	UNP Q9Z8J2
A	565	PRO	-	expression tag	UNP Q9Z8J2
A	566	GLN	-	expression tag	UNP Q9Z8J2
A	567	PHE	-	expression tag	UNP Q9Z8J2
A	568	GLU	-	expression tag	UNP Q9Z8J2
A	569	LYS	-	expression tag	UNP Q9Z8J2
A	570	GLY	-	expression tag	UNP Q9Z8J2
A	571	GLY	-	expression tag	UNP Q9Z8J2
A	572	GLY	-	expression tag	UNP Q9Z8J2
A	573	GLY	-	expression tag	UNP Q9Z8J2
A	574	SER	-	expression tag	UNP Q9Z8J2
A	575	GLY	-	expression tag	UNP Q9Z8J2
A	576	GLY	-	expression tag	UNP Q9Z8J2
A	577	SER	-	expression tag	UNP Q9Z8J2
A	578	ALA	-	expression tag	UNP Q9Z8J2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	579	TRP	-	expression tag	UNP Q9Z8J2
A	580	SER	-	expression tag	UNP Q9Z8J2
A	581	HIS	-	expression tag	UNP Q9Z8J2
A	582	PRO	-	expression tag	UNP Q9Z8J2
A	583	GLN	-	expression tag	UNP Q9Z8J2
A	584	PHE	-	expression tag	UNP Q9Z8J2
A	585	GLU	-	expression tag	UNP Q9Z8J2
A	586	LYS	-	expression tag	UNP Q9Z8J2

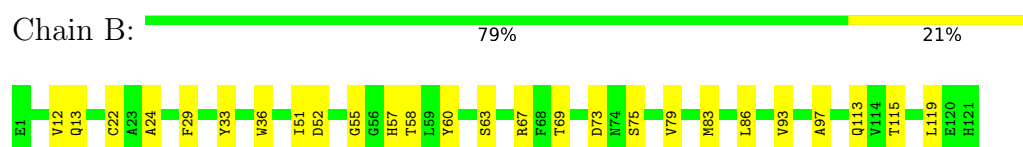
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



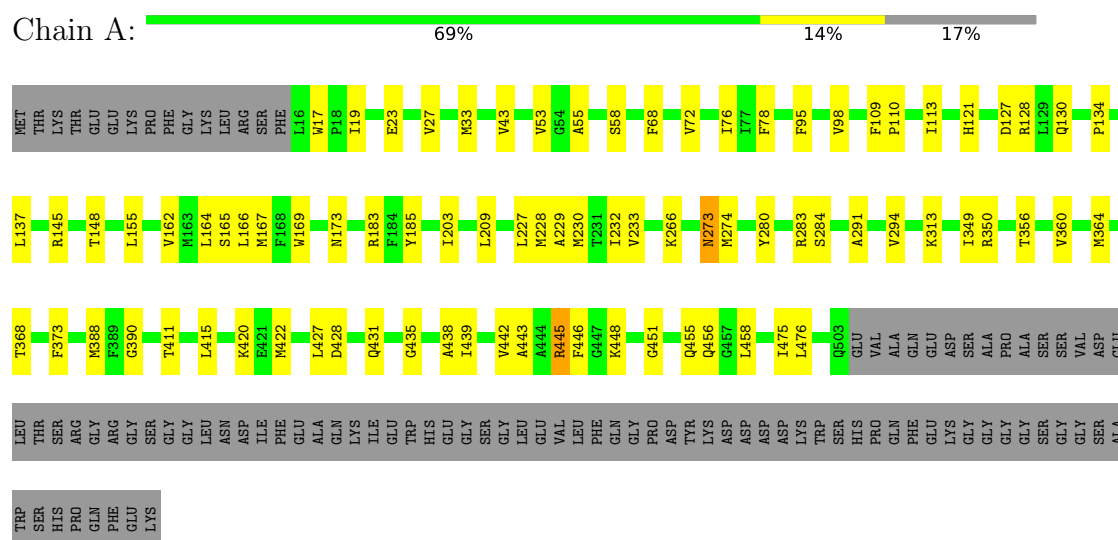
3 Residue-property plots

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: 1D10



• Molecule 2: ADP,ATP carrier protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119152	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (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: 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	B	0.16	0/972	0.35	0/1315
2	A	0.19	0/3929	0.37	0/5340
All	All	0.19	0/4901	0.36	0/6655

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	B	949	0	892	18	0
2	A	3829	0	4019	57	0
3	A	31	0	12	2	0
All	All	4809	0	4923	74	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 8.

All (74) 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:B:113:GLN:HE22	1:B:115:THR:HB	1.52	0.75
2:A:445:ARG:O	2:A:446:PHE:C	2.35	0.69
1:B:51:ILE:HD11	1:B:55:GLY:HA2	1.77	0.66
1:B:12:VAL:HG23	1:B:13:GLN:H	1.61	0.65
3:A:601:ATP:H4'	3:A:601:ATP:O2A	1.99	0.62
1:B:52:ASP:HB2	1:B:57:HIS:HB3	1.82	0.62
2:A:43:VAL:HA	2:A:203:ILE:HD11	1.81	0.61
2:A:428:ASP:H	2:A:431:GLN:HE21	1.47	0.61
1:B:29:PHE:HZ	1:B:79:VAL:HG23	1.66	0.60
1:B:63:SER:O	1:B:67:ARG:NH2	2.33	0.60
2:A:458:LEU:HD11	2:A:475:ILE:HD12	1.84	0.60
2:A:164:LEU:HD23	3:A:601:ATP:O2'	2.02	0.60
2:A:165:SER:HA	2:A:169:TRP:HD1	1.69	0.58
2:A:294:VAL:HG22	2:A:420:LYS:HD2	1.85	0.57
1:B:51:ILE:HD12	1:B:58:THR:HG22	1.86	0.57
2:A:438:ALA:O	2:A:442:VAL:HG22	2.04	0.57
2:A:121:HIS:NE2	2:A:148:THR:OG1	2.31	0.56
2:A:283:ARG:HG3	2:A:284:SER:N	2.20	0.56
2:A:17:TRP:CZ2	2:A:19:ILE:HD11	2.41	0.56
2:A:435:GLY:O	2:A:439:ILE:HG12	2.06	0.55
2:A:411:THR:HB	2:A:415:LEU:HD12	1.88	0.55
2:A:19:ILE:HD12	2:A:27:VAL:HG11	1.89	0.54
2:A:373:PHE:HE2	2:A:476:LEU:HD13	1.73	0.54
1:B:22:CYS:HB3	1:B:79:VAL:HB	1.90	0.54
2:A:72:VAL:O	2:A:76:ILE:HG12	2.07	0.53
1:B:83:MET:HB3	1:B:86:LEU:HD21	1.91	0.53
2:A:130:GLN:OE1	2:A:145:ARG:NH2	2.42	0.52
2:A:280:TYR:O	2:A:283:ARG:HG2	2.08	0.52
2:A:227:LEU:HA	2:A:230:MET:HE2	1.91	0.51
1:B:33:TYR:CZ	1:B:52:ASP:HA	2.47	0.50
2:A:356:THR:O	2:A:360:VAL:HG23	2.11	0.50
1:B:57:HIS:NE2	2:A:390:GLY:O	2.38	0.50
1:B:36:TRP:HE1	1:B:79:VAL:HG12	1.76	0.49
2:A:349:ILE:HG13	2:A:350:ARG:N	2.27	0.49
2:A:165:SER:O	2:A:169:TRP:HB2	2.13	0.49
2:A:68:PHE:HB3	2:A:456:GLN:HE22	1.78	0.48
2:A:55:ALA:HB3	2:A:58:SER:HB3	1.95	0.48
2:A:109:PHE:HA	2:A:113:ILE:HB	1.96	0.48
2:A:209:LEU:O	2:A:209:LEU:HD23	2.14	0.47
1:B:73:ASP:OD2	1:B:75:SER:OG	2.25	0.47
1:B:97:ALA:HB3	2:A:388:MET:HE3	1.97	0.46
2:A:110:PRO:HG3	2:A:228:MET:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HD23	1:B:119:LEU:H	1.79	0.46
2:A:162:VAL:HG12	2:A:167:MET:HG2	1.96	0.46
2:A:127:ASP:OD1	2:A:128:ARG:N	2.48	0.46
2:A:78:PHE:HZ	2:A:98:VAL:HG13	1.80	0.46
2:A:162:VAL:HG13	2:A:166:LEU:HD23	1.97	0.46
2:A:445:ARG:CD	2:A:448:LYS:HE3	2.46	0.45
2:A:364:MET:O	2:A:368:THR:OG1	2.32	0.45
2:A:155:LEU:HD23	2:A:155:LEU:HA	1.83	0.45
2:A:445:ARG:HD3	2:A:448:LYS:HE3	1.99	0.45
2:A:349:ILE:HG13	2:A:350:ARG:H	1.81	0.44
2:A:273:ASN:OD1	2:A:274:MET:N	2.47	0.44
2:A:442:VAL:HG23	2:A:443:ALA:N	2.33	0.44
2:A:134:PRO:HD2	2:A:137:LEU:HD12	1.99	0.44
2:A:68:PHE:O	2:A:72:VAL:HG22	2.17	0.44
2:A:445:ARG:O	2:A:448:LYS:N	2.51	0.44
2:A:228:MET:O	2:A:232:ILE:HG12	2.18	0.43
2:A:266:LYS:HA	2:A:266:LYS:HD2	1.85	0.42
2:A:229:ALA:O	2:A:233:VAL:HG23	2.19	0.42
2:A:53:VAL:CG1	2:A:313:LYS:HB2	2.50	0.42
2:A:173:ASN:OD1	2:A:185:TYR:OH	2.25	0.42
2:A:23:GLU:CD	2:A:183:ARG:HH22	2.27	0.42
2:A:33:MET:HE2	2:A:33:MET:HB3	1.93	0.41
2:A:451:GLY:O	2:A:455:GLN:HG3	2.19	0.41
1:B:93:VAL:HA	1:B:113:GLN:HA	2.01	0.41
2:A:291:ALA:HB2	2:A:439:ILE:HD12	2.02	0.41
1:B:60:TYR:CE1	1:B:69:THR:HA	2.56	0.41
1:B:22:CYS:O	1:B:24:ALA:N	2.54	0.41
2:A:349:ILE:HD12	2:A:422:MET:HE1	2.02	0.41
2:A:95:PHE:HA	2:A:167:MET:HE2	2.02	0.40
2:A:364:MET:HE3	2:A:364:MET:HB3	1.97	0.40
2:A:17:TRP:CE2	2:A:19:ILE:HD11	2.56	0.40
2:A:427:LEU:HB3	2:A:431:GLN:HG3	2.04	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	B	119/121 (98%)	104 (87%)	15 (13%)	0	100	100
2	A	486/586 (83%)	456 (94%)	29 (6%)	1 (0%)	44	67
All	All	605/707 (86%)	560 (93%)	44 (7%)	1 (0%)	45	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	273	ASN

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	B	99/99 (100%)	99 (100%)	0	100	100
2	A	407/486 (84%)	406 (100%)	1 (0%)	92	98
All	All	506/585 (86%)	505 (100%)	1 (0%)	91	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	445	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	39	GLN
1	B	77	ASN
1	B	82	GLN
1	B	113	GLN

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Mol	Chain	Res	Type
2	A	20	HIS
2	A	404	GLN
2	A	431	GLN

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](#)

1 ligand is 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	$\# Z > 2$
3	ATP	A	601	-	26,33,33	0.98	1 (3%)	31,52,52	1.84	6 (19%)

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	ATP	A	601	-	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ATP	C5-C4	2.43	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ATP	PA-O3A-PB	-5.51	113.92	132.83
3	A	601	ATP	C3'-C2'-C1'	3.83	106.75	100.98
3	A	601	ATP	N3-C2-N1	-3.40	123.36	128.68
3	A	601	ATP	PB-O3B-PG	-3.31	121.46	132.83
3	A	601	ATP	C4-C5-N7	-2.15	107.16	109.40
3	A	601	ATP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

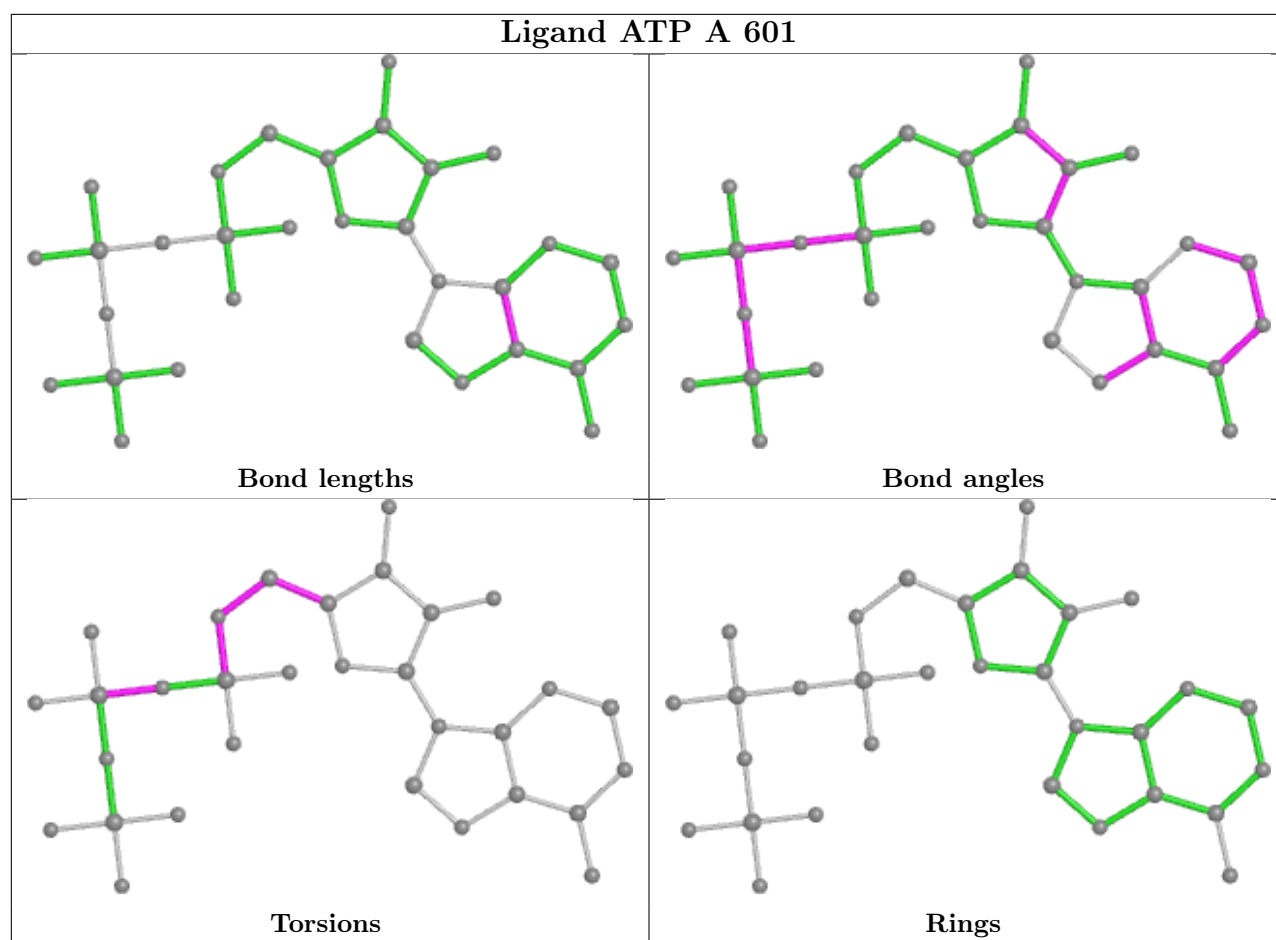
Mol	Chain	Res	Type	Atoms
3	A	601	ATP	C4'-C5'-O5'-PA
3	A	601	ATP	C3'-C4'-C5'-O5'
3	A	601	ATP	O4'-C4'-C5'-O5'
3	A	601	ATP	PA-O3A-PB-O1B
3	A	601	ATP	C5'-O5'-PA-O2A
3	A	601	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ATP	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.