



## Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 01:59 AM JST

PDB ID : 9J3L / pdb\_00009j3l  
EMDB ID : EMD-61118  
Title : ATP bound Arabidopsis ATP/ADP translocator AtNTT1  
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](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) : 2.44

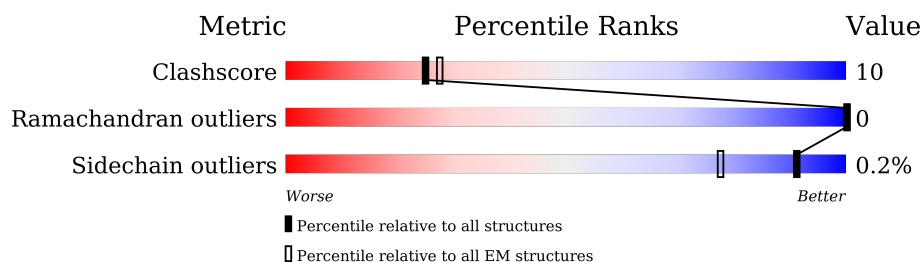
# 1 Overall quality at a glance

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  $\geq 3$ , 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	610	
2	C	120	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4730 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 ADP,ATP carrier protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	482	Total	C	N	O	S	1	0
			3750	2507	580	639	24		

There are 73 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	MET	-	initiating methionine	UNP Q39002
A	87	ALA	-	expression tag	UNP Q39002
A	625	VAL	-	expression tag	UNP Q39002
A	626	ASP	-	expression tag	UNP Q39002
A	627	GLU	-	expression tag	UNP Q39002
A	628	LEU	-	expression tag	UNP Q39002
A	629	THR	-	expression tag	UNP Q39002
A	630	SER	-	expression tag	UNP Q39002
A	631	ARG	-	expression tag	UNP Q39002
A	632	GLY	-	expression tag	UNP Q39002
A	633	ARG	-	expression tag	UNP Q39002
A	634	GLY	-	expression tag	UNP Q39002
A	635	SER	-	expression tag	UNP Q39002
A	636	GLY	-	expression tag	UNP Q39002
A	637	GLY	-	expression tag	UNP Q39002
A	638	LEU	-	expression tag	UNP Q39002
A	639	ASN	-	expression tag	UNP Q39002
A	640	ASP	-	expression tag	UNP Q39002
A	641	ILE	-	expression tag	UNP Q39002
A	642	PHE	-	expression tag	UNP Q39002
A	643	GLU	-	expression tag	UNP Q39002
A	644	ALA	-	expression tag	UNP Q39002
A	645	GLN	-	expression tag	UNP Q39002
A	646	LYS	-	expression tag	UNP Q39002
A	647	ILE	-	expression tag	UNP Q39002
A	648	GLU	-	expression tag	UNP Q39002
A	649	TRP	-	expression tag	UNP Q39002
A	650	HIS	-	expression tag	UNP Q39002

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Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	-	expression tag	UNP Q39002
A	652	GLY	-	expression tag	UNP Q39002
A	653	SER	-	expression tag	UNP Q39002
A	654	GLY	-	expression tag	UNP Q39002
A	655	LEU	-	expression tag	UNP Q39002
A	656	GLU	-	expression tag	UNP Q39002
A	657	VAL	-	expression tag	UNP Q39002
A	658	LEU	-	expression tag	UNP Q39002
A	659	PHE	-	expression tag	UNP Q39002
A	660	GLN	-	expression tag	UNP Q39002
A	661	GLY	-	expression tag	UNP Q39002
A	662	PRO	-	expression tag	UNP Q39002
A	663	ASP	-	expression tag	UNP Q39002
A	664	TYR	-	expression tag	UNP Q39002
A	665	LYS	-	expression tag	UNP Q39002
A	666	ASP	-	expression tag	UNP Q39002
A	667	ASP	-	expression tag	UNP Q39002
A	668	ASP	-	expression tag	UNP Q39002
A	669	ASP	-	expression tag	UNP Q39002
A	670	LYS	-	expression tag	UNP Q39002
A	671	TRP	-	expression tag	UNP Q39002
A	672	SER	-	expression tag	UNP Q39002
A	673	HIS	-	expression tag	UNP Q39002
A	674	PRO	-	expression tag	UNP Q39002
A	675	GLN	-	expression tag	UNP Q39002
A	676	PHE	-	expression tag	UNP Q39002
A	677	GLU	-	expression tag	UNP Q39002
A	678	LYS	-	expression tag	UNP Q39002
A	679	GLY	-	expression tag	UNP Q39002
A	680	GLY	-	expression tag	UNP Q39002
A	681	GLY	-	expression tag	UNP Q39002
A	682	GLY	-	expression tag	UNP Q39002
A	683	SER	-	expression tag	UNP Q39002
A	684	GLY	-	expression tag	UNP Q39002
A	685	GLY	-	expression tag	UNP Q39002
A	686	SER	-	expression tag	UNP Q39002
A	687	ALA	-	expression tag	UNP Q39002
A	688	TRP	-	expression tag	UNP Q39002
A	689	SER	-	expression tag	UNP Q39002
A	690	HIS	-	expression tag	UNP Q39002
A	691	PRO	-	expression tag	UNP Q39002
A	692	GLN	-	expression tag	UNP Q39002

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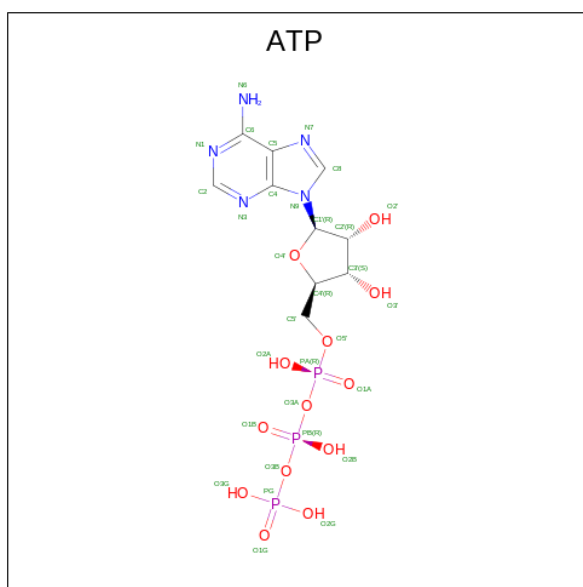
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Chain	Residue	Modelled	Actual	Comment	Reference
A	693	PHE	-	expression tag	UNP Q39002
A	694	GLU	-	expression tag	UNP Q39002
A	695	LYS	-	expression tag	UNP Q39002

- Molecule 2 is a protein called nanobody: B-D7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	120	Total	C	N	O	S	0	0
			949	600	157	188	4		

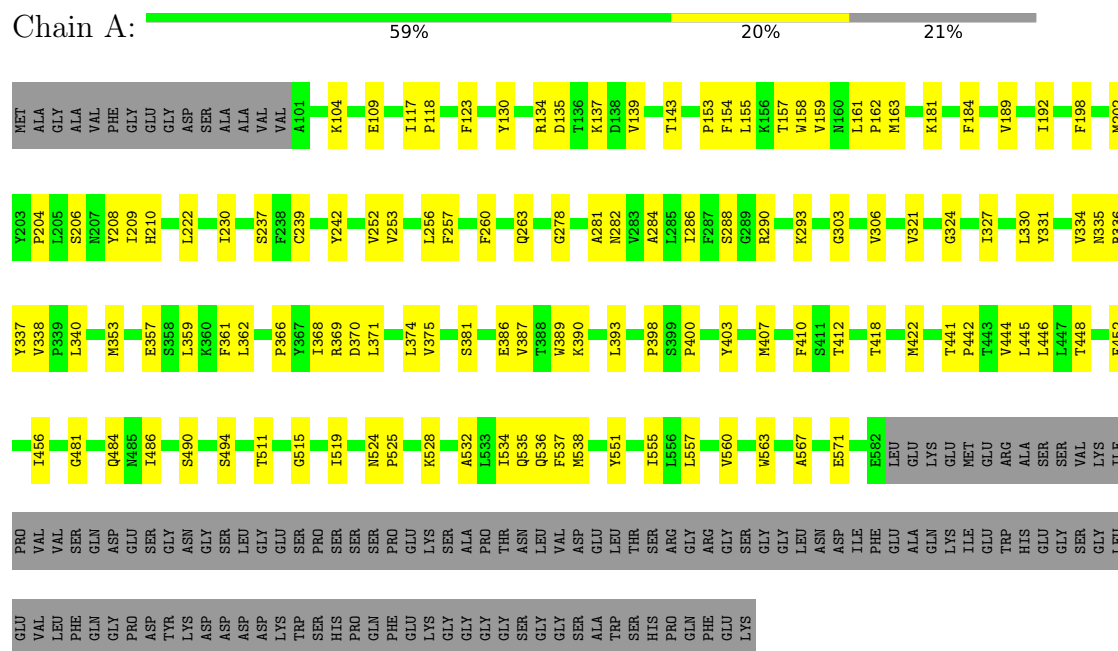
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



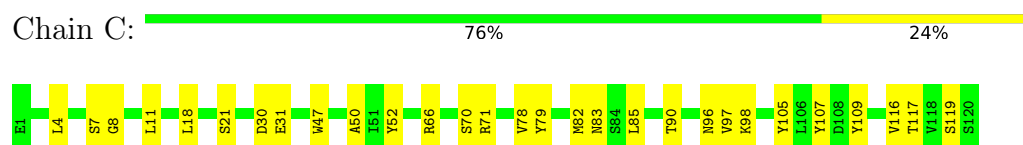
### 3 Residue-property plots

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: ADP,ATP carrier protein 1, chloroplastic



- Molecule 2: nanobody: B-D7



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	679696	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 ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k 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: 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	0.14	0/3854	0.39	1/5236 (0.0%)
2	C	0.09	0/972	0.26	0/1321
All	All	0.13	0/4826	0.37	1/6557 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	TYR	N-CA-C	-6.43	106.39	114.56

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	3750	0	3912	80	0
2	C	949	0	896	18	0
3	A	31	0	12	5	0
All	All	4730	0	4820	98	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 10.



All (98) 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:198:PHE:HA	1:A:202:MET:HB2	1.67	0.74
1:A:353:MET:HE3	1:A:357:GLU:HG3	1.73	0.70
1:A:210:HIS:NE2	1:A:237:SER:OG	2.23	0.70
1:A:143:THR:HG22	1:A:143:THR:O	1.93	0.67
1:A:515:GLY:O	1:A:519:ILE:HG12	1.96	0.66
1:A:143:THR:HG23	1:A:398:PRO:O	1.97	0.65
1:A:324:GLY:HA2	1:A:327:ILE:HD12	1.79	0.65
2:C:82:MET:HE1	2:C:116:VAL:HG11	1.77	0.65
1:A:567:ALA:O	1:A:571:GLU:N	2.27	0.65
1:A:442:PRO:HG3	1:A:563:TRP:CE2	2.32	0.65
1:A:386:GLU:HG2	1:A:390:LYS:HE3	1.78	0.64
1:A:139:VAL:HG22	1:A:403:TYR:HD1	1.61	0.63
1:A:181:LYS:HE2	1:A:335:ASN:HB3	1.80	0.62
2:C:52:TYR:O	2:C:71:ARG:NH1	2.29	0.61
1:A:528:LYS:NZ	3:A:701:ATP:O1B	2.35	0.60
2:C:70:SER:O	2:C:79:TYR:N	2.28	0.59
2:C:82:MET:HB3	2:C:85:LEU:HD21	1.84	0.59
1:A:157:THR:HB	1:A:536:GLN:HE22	1.68	0.58
2:C:11:LEU:HD11	2:C:119:SER:HB3	1.85	0.58
1:A:134:ARG:NH2	3:A:701:ATP:O2G	2.38	0.57
1:A:331:TYR:O	1:A:335:ASN:ND2	2.32	0.56
1:A:303:GLY:HA3	1:A:306:VAL:HB	1.87	0.56
2:C:30:ASP:OD1	2:C:31:GLU:HG2	2.06	0.56
1:A:290:ARG:HH21	1:A:293:LYS:HD3	1.71	0.55
1:A:387:VAL:HB	1:A:535:GLN:HE22	1.71	0.55
1:A:361:PHE:HZ	1:A:511:THR:HG23	1.70	0.55
1:A:153:PRO:HA	1:A:532:ALA:HB1	1.88	0.55
2:C:47:TRP:HE1	2:C:50:ALA:HB2	1.71	0.54
2:C:90:THR:HG23	2:C:117:THR:HA	1.90	0.54
1:A:252:VAL:HA	1:A:256:LEU:HB2	1.90	0.53
1:A:381:SER:HB3	1:A:445:LEU:HD21	1.89	0.53
1:A:446:LEU:HD22	1:A:560:VAL:HG11	1.90	0.53
1:A:104:LYS:HG2	1:A:109:GLU:HA	1.91	0.53
1:A:418:THR:O	1:A:422:MET:HG3	2.09	0.53
1:A:452:PHE:CZ	1:A:456:ILE:HD11	2.43	0.52
1:A:189:VAL:HA	1:A:192:ILE:HD12	1.93	0.51
1:A:143:THR:O	1:A:143:THR:CG2	2.59	0.51
1:A:184:PHE:CE2	1:A:256:LEU:HB3	2.46	0.51
1:A:524:ASN:HB3	1:A:525:PRO:HD3	1.90	0.51
1:A:192:ILE:HG23	1:A:321:VAL:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HA	1:A:362:LEU:HB2	1.94	0.50
2:C:107:TYR:HB2	2:C:109:TYR:CE1	2.47	0.50
1:A:390:LYS:HA	1:A:393:LEU:HD12	1.94	0.49
1:A:155:LEU:HD23	1:A:159:VAL:HG21	1.94	0.49
2:C:98:LYS:HD2	2:C:105:TYR:HE2	1.77	0.49
2:C:71:ARG:HA	2:C:78:VAL:HA	1.95	0.49
1:A:130:TYR:OH	3:A:701:ATP:H5'1	2.12	0.48
1:A:389:TRP:CD1	1:A:481:GLY:HA3	2.48	0.48
1:A:537:PHE:HD2	1:A:538:MET:HE2	1.78	0.48
1:A:222:LEU:HD12	1:A:230:ILE:HD11	1.94	0.48
1:A:441:THR:HA	1:A:444:VAL:HG12	1.95	0.48
1:A:532:ALA:O	1:A:536:GLN:HG3	2.14	0.48
2:C:82:MET:HE2	2:C:85:LEU:HD21	1.96	0.48
2:C:7:SER:OG	2:C:21:SER:OG	2.32	0.48
1:A:370:ASP:O	1:A:374:LEU:HG	2.14	0.47
1:A:284:ALA:O	1:A:288:SER:OG	2.31	0.47
1:A:260:PHE:HA	1:A:263:GLN:HG2	1.96	0.46
1:A:143:THR:HG21	1:A:400:PRO:N	2.30	0.46
2:C:8:GLY:O	2:C:18:LEU:HD11	2.16	0.46
2:C:96:ASN:ND2	2:C:109:TYR:O	2.45	0.46
1:A:130:TYR:OH	3:A:701:ATP:O3A	2.34	0.45
1:A:334:VAL:O	1:A:338:VAL:HB	2.16	0.45
1:A:290:ARG:HH21	1:A:293:LYS:CD	2.30	0.45
1:A:448:THR:OG1	1:A:484:GLN:HG2	2.17	0.45
1:A:330:LEU:O	1:A:334:VAL:HG23	2.16	0.45
1:A:410:PHE:CE1	1:A:486:ILE:HG13	2.51	0.45
1:A:158:TRP:NE1	1:A:536:GLN:OE1	2.50	0.44
1:A:441:THR:HB	1:A:442:PRO:HD3	1.98	0.44
2:C:4:LEU:HD11	2:C:97:VAL:HG12	1.98	0.44
1:A:184:PHE:HD1	1:A:184:PHE:O	2.01	0.44
1:A:206:SER:HA	1:A:209:ILE:HG12	1.99	0.44
1:A:446:LEU:HD21	1:A:557:LEU:HD13	2.00	0.43
1:A:490:SER:O	1:A:494:SER:OG	2.30	0.43
1:A:368:ILE:HG23	1:A:519:ILE:HD11	2.00	0.43
1:A:123:PHE:HB2	1:A:257:PHE:CZ	2.54	0.43
1:A:154:PHE:HA	1:A:536:GLN:NE2	2.34	0.43
1:A:290:ARG:NH1	1:A:412:THR:HG21	2.34	0.43
2:C:107:TYR:HB2	2:C:109:TYR:HE1	1.84	0.42
1:A:340:LEU:HD23	1:A:340:LEU:H	1.84	0.42
1:A:134:ARG:HG3	1:A:137:LYS:NZ	2.35	0.42
1:A:286:ILE:HG23	1:A:412:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:TRP:O	1:A:393:LEU:HG	2.20	0.42
1:A:366:PRO:HA	1:A:369:ARG:HG2	2.02	0.42
1:A:371:LEU:O	1:A:375:VAL:HG23	2.19	0.41
1:A:161:LEU:HB3	1:A:162:PRO:HD3	2.02	0.41
1:A:123:PHE:CE2	1:A:281:ALA:HB2	2.56	0.41
1:A:137:LYS:HE2	1:A:242:TYR:CZ	2.56	0.41
1:A:163:MET:HE3	1:A:163:MET:HB3	1.93	0.41
1:A:278:GLY:O	1:A:282:ASN:ND2	2.54	0.41
1:A:117:ILE:HB	1:A:118:PRO:HD3	2.02	0.41
1:A:253:VAL:HG11	3:A:701:ATP:H1'	2.02	0.41
1:A:336:ARG:NH1	1:A:337:TYR:CE1	2.88	0.41
1:A:551:TYR:O	1:A:555:ILE:HD12	2.20	0.41
1:A:135:ASP:HB3	1:A:407:MET:HB3	2.03	0.41
1:A:155:LEU:HD21	1:A:239:CYS:SG	2.61	0.41
2:C:66:ARG:HB3	2:C:83:ASN:O	2.21	0.40
1:A:534:ILE:O	1:A:538:MET:HG2	2.22	0.40
1:A:135:ASP:O	1:A:139:VAL:HG23	2.22	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	481/610 (79%)	451 (94%)	30 (6%)	0	100	100
2	C	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
All	All	599/730 (82%)	568 (95%)	31 (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	406/506 (80%)	404 (100%)	2 (0%)	86	95
2	C	100/100 (100%)	100 (100%)	0	100	100
All	All	506/606 (84%)	504 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204[A]	PRO
1	A	204[B]	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	ASN
1	A	535	GLN
1	A	573	GLN
2	C	81	GLN
2	C	83	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

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	701	-	26,33,33	1.12	1 (3%)	31,52,52	1.52	5 (16%)

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	701	-	-	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	701	ATP	C5-N7	-2.07	1.32	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ATP	O5'-C5'-C4'	3.66	121.57	108.99
3	A	701	ATP	C4-C5-N7	-3.05	106.22	109.40
3	A	701	ATP	PB-O3B-PG	-2.77	123.31	132.83
3	A	701	ATP	N3-C2-N1	-2.24	125.18	128.68
3	A	701	ATP	C2'-C3'-C4'	2.06	106.64	102.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	ATP	C5'-O5'-PA-O3A
3	A	701	ATP	C3'-C4'-C5'-O5'

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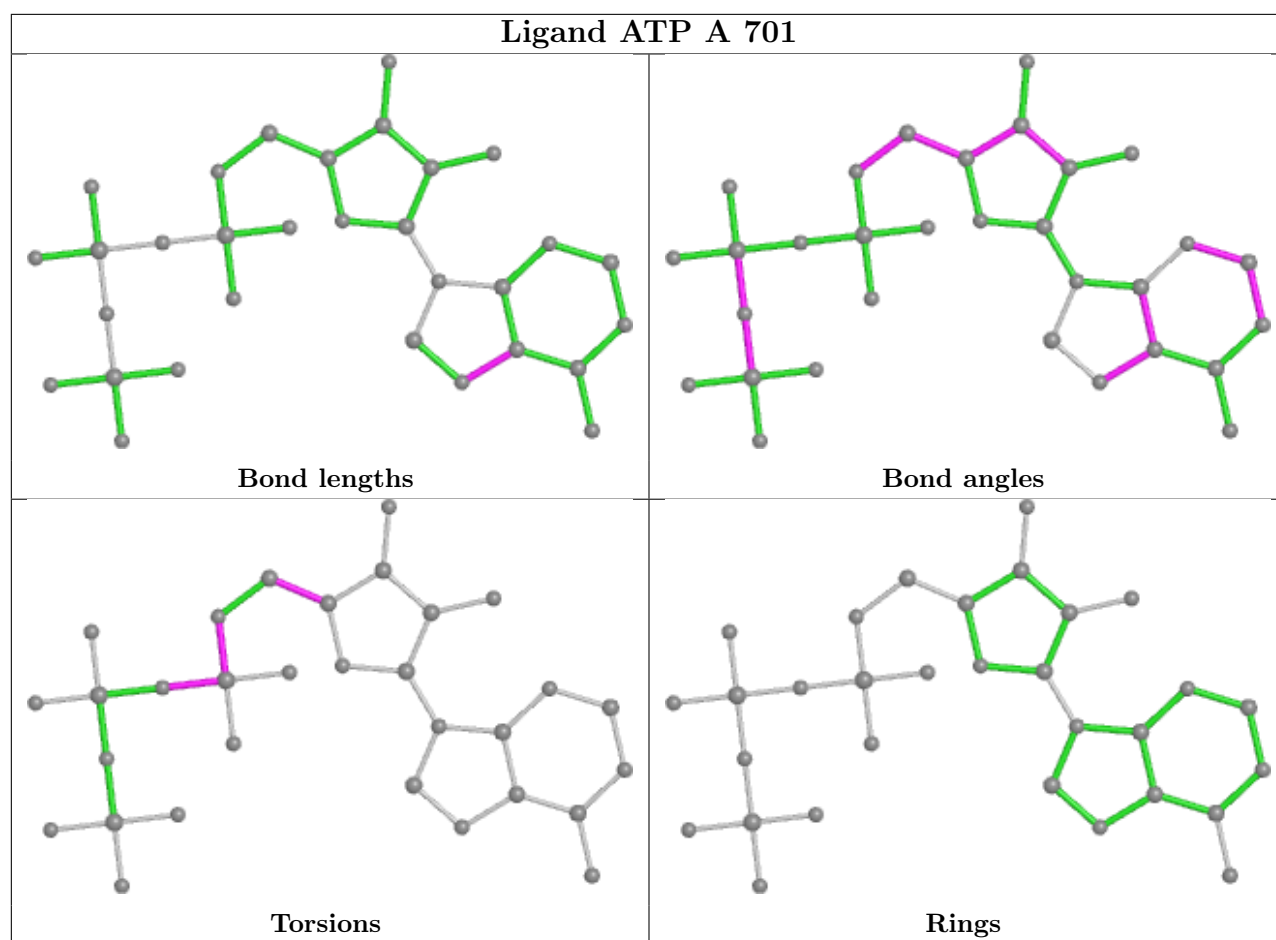
Mol	Chain	Res	Type	Atoms
3	A	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	PB-O3A-PA-O2A
3	A	701	ATP	C5'-O5'-PA-O1A
3	A	701	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	ATP	5	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.