



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 17, 2024 – 07:56 PM EST

PDB ID : 3TY5  
Title : Crystal Structure of *C. thermocellum* PNKP Ligase domain in complex with ATP  
Authors : Smith, P.; Wang, L.; Shuman, S.  
Deposited on : 2011-09-23  
Resolution : 2.40 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

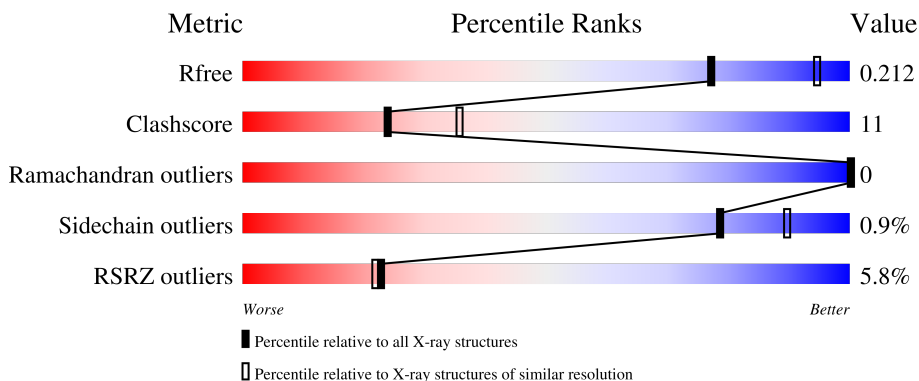
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	413	 5% 72% 20% 8%
1	B	413	 6% 75% 17% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PGE	B	1	-	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6381 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Polynucleotide 2',3'-cyclic phosphate phosphodiesterase / polynucleotide 5'-hydroxyl-kinase / polynucleotide 3'-phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	3057	1935	535	564	23	0	0	0
1	B	381	3043	1928	529	565	21	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

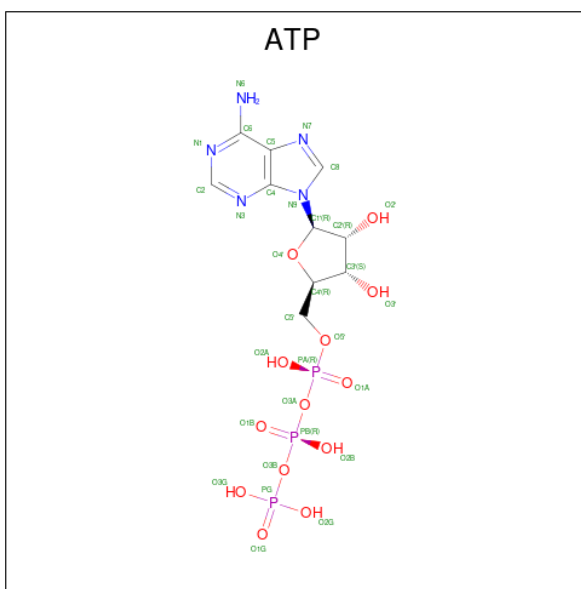
Chain	Residue	Modelled	Actual	Comment	Reference
A	458	MET	-	expression tag	UNP A3DJ38
A	459	GLY	-	expression tag	UNP A3DJ38
A	460	HIS	-	expression tag	UNP A3DJ38
A	461	HIS	-	expression tag	UNP A3DJ38
A	462	HIS	-	expression tag	UNP A3DJ38
A	463	HIS	-	expression tag	UNP A3DJ38
A	464	HIS	-	expression tag	UNP A3DJ38
A	465	HIS	-	expression tag	UNP A3DJ38
A	466	HIS	-	expression tag	UNP A3DJ38
A	467	HIS	-	expression tag	UNP A3DJ38
A	468	HIS	-	expression tag	UNP A3DJ38
A	469	HIS	-	expression tag	UNP A3DJ38
A	470	SER	-	expression tag	UNP A3DJ38
A	471	SER	-	expression tag	UNP A3DJ38
A	472	GLY	-	expression tag	UNP A3DJ38
A	473	HIS	-	expression tag	UNP A3DJ38
A	474	ILE	-	expression tag	UNP A3DJ38
A	475	GLU	-	expression tag	UNP A3DJ38
A	476	GLY	-	expression tag	UNP A3DJ38
A	477	ARG	-	expression tag	UNP A3DJ38
A	478	HIS	-	expression tag	UNP A3DJ38
A	529	GLY	GLU	engineered mutation	UNP A3DJ38
B	458	MET	-	expression tag	UNP A3DJ38
B	459	GLY	-	expression tag	UNP A3DJ38

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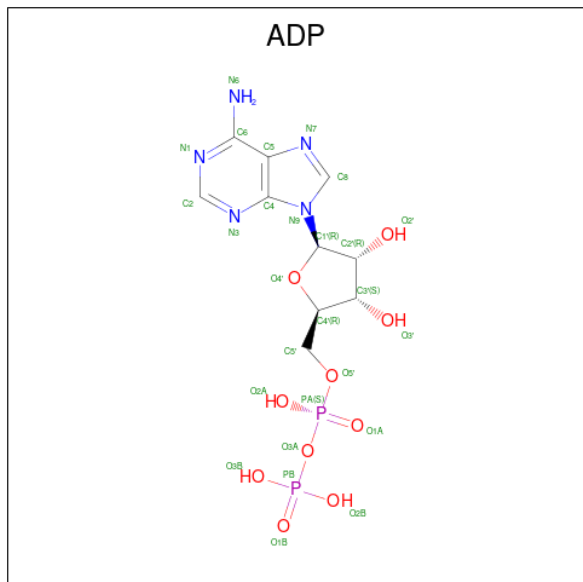
Chain	Residue	Modelled	Actual	Comment	Reference
B	460	HIS	-	expression tag	UNP A3DJ38
B	461	HIS	-	expression tag	UNP A3DJ38
B	462	HIS	-	expression tag	UNP A3DJ38
B	463	HIS	-	expression tag	UNP A3DJ38
B	464	HIS	-	expression tag	UNP A3DJ38
B	465	HIS	-	expression tag	UNP A3DJ38
B	466	HIS	-	expression tag	UNP A3DJ38
B	467	HIS	-	expression tag	UNP A3DJ38
B	468	HIS	-	expression tag	UNP A3DJ38
B	469	HIS	-	expression tag	UNP A3DJ38
B	470	SER	-	expression tag	UNP A3DJ38
B	471	SER	-	expression tag	UNP A3DJ38
B	472	GLY	-	expression tag	UNP A3DJ38
B	473	HIS	-	expression tag	UNP A3DJ38
B	474	ILE	-	expression tag	UNP A3DJ38
B	475	GLU	-	expression tag	UNP A3DJ38
B	476	GLY	-	expression tag	UNP A3DJ38
B	477	ARG	-	expression tag	UNP A3DJ38
B	478	HIS	-	expression tag	UNP A3DJ38
B	529	GLY	GLU	engineered mutation	UNP A3DJ38

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



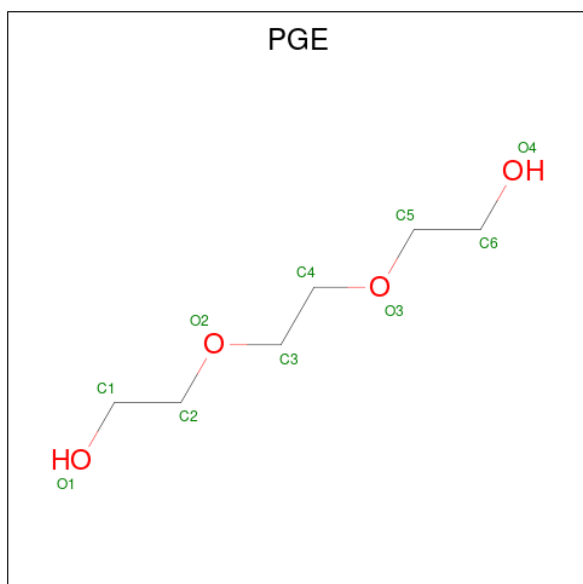
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	27	10	5	10	2	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	10	6	4	0	0

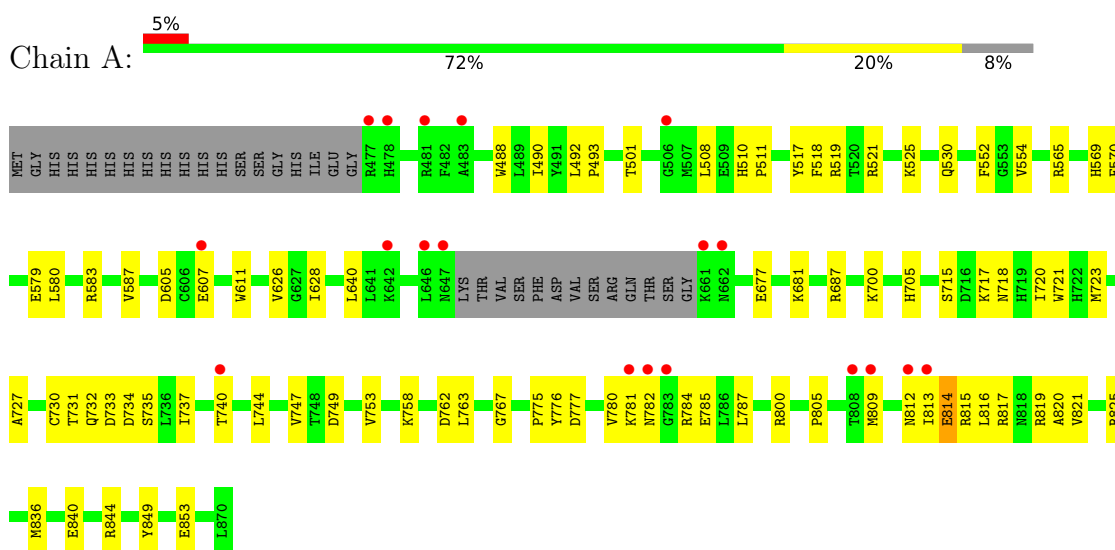
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	117	Total 117	O 117	0	0
5	B	96	Total 96	O 96	0	0

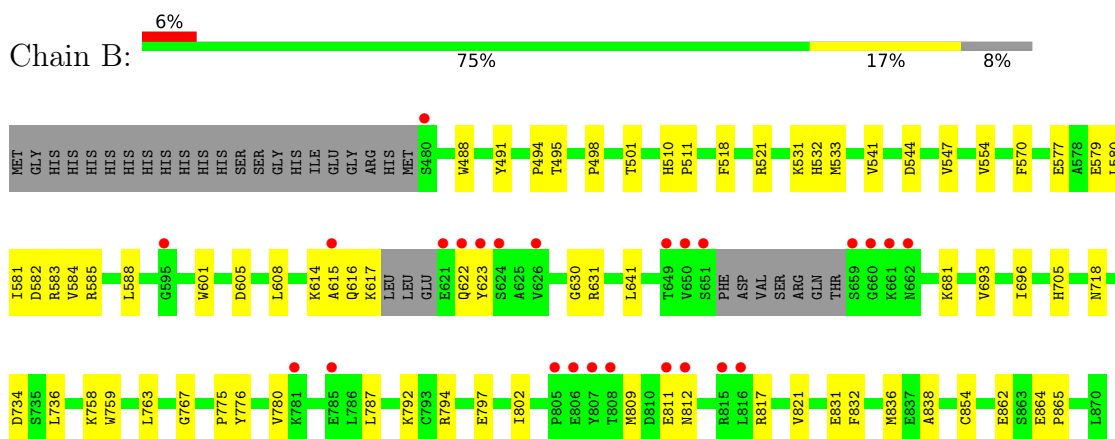
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Polynucleotide 2',3'-cyclic phosphate phosphodiesterase / polynucleotide 5'-hydroxyl-kinase / polynucleotide 3'-phosphatase



- Molecule 1: Polynucleotide 2',3'-cyclic phosphate phosphodiesterase / polynucleotide 5'-hydroxyl-kinase / polynucleotide 3'-phosphatase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.99Å 94.38Å 75.31Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	44.33 – 2.40 39.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (44.33-2.40) 99.2 (39.97-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.178 , 0.225 0.170 , 0.212	Depositor DCC
$R_{free}$ test set	1571 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtrriage
Anisotropy	0.167	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, PGE, ADP

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	0.29	0/3122	0.46	0/4213
1	B	0.28	0/3107	0.43	0/4192
All	All	0.28	0/6229	0.45	0/8405

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	3057	0	3020	80	0
1	B	3043	0	3004	59	0
2	A	31	0	10	0	0
3	B	27	0	12	2	0
4	B	10	0	14	8	0
5	A	117	0	0	6	0
5	B	96	0	0	4	0
All	All	6381	0	6060	136	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.

The worst 5 of 136 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:616:GLN:HG2	1:B:617:LYS:H	1.23	1.03
1:A:501:THR:HG21	1:A:815:ARG:HG3	1.43	1.01
1:B:491:TYR:HE1	4:B:1:PGE:H5	1.23	0.99
1:B:498:PRO:HB3	1:B:794:ARG:HH12	1.29	0.97
1:B:832:PHE:HA	4:B:1:PGE:H62	1.47	0.96

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 X-ray entries followed by that with respect to entries of similar resolution.

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	377/413 (91%)	362 (96%)	15 (4%)	0	100	100
1	B	375/413 (91%)	364 (97%)	11 (3%)	0	100	100
All	All	752/826 (91%)	726 (96%)	26 (4%)	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 X-ray entries followed by that with respect to entries of similar resolution.

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	329/360 (91%)	323 (98%)	6 (2%)	59	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	328/360 (91%)	328 (100%)	0	100	100
All	All	657/720 (91%)	651 (99%)	6 (1%)	78	90

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	733	ASP
1	A	809	MET
1	A	814	GLU
1	A	570	PHE
1	A	569	HIS

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	569	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	ATP	A	1001	-	26,33,33	1.79	6 (23%)	31,52,52	2.58	15 (48%)
3	ADP	B	1001	-	24,29,29	2.14	7 (29%)	29,45,45	2.23	10 (34%)
4	PGE	B	1	-	9,9,9	0.57	0	8,8,8	1.38	1 (12%)

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	ATP	A	1001	-	-	8/18/38/38	0/3/3/3
3	ADP	B	1001	-	-	4/12/32/32	0/3/3/3
4	PGE	B	1	-	-	4/7/7/7	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ATP	O4'-C1'	5.25	1.48	1.41
3	B	1001	ADP	C5-C4	5.20	1.54	1.40
3	B	1001	ADP	C4-N3	4.22	1.41	1.35
3	B	1001	ADP	C2-N1	3.80	1.41	1.33
3	B	1001	ADP	C2'-C1'	3.33	1.58	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ATP	N6-C6-N1	6.32	131.70	118.57
2	A	1001	ATP	C5-C6-N6	-5.02	112.72	120.35
3	B	1001	ADP	C4-C5-N7	-4.48	104.73	109.40
3	B	1001	ADP	C3'-C2'-C1'	4.34	107.51	100.98
2	A	1001	ATP	O2'-C2'-C3'	4.07	124.97	111.82

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	C5'-O5'-PA-O1A

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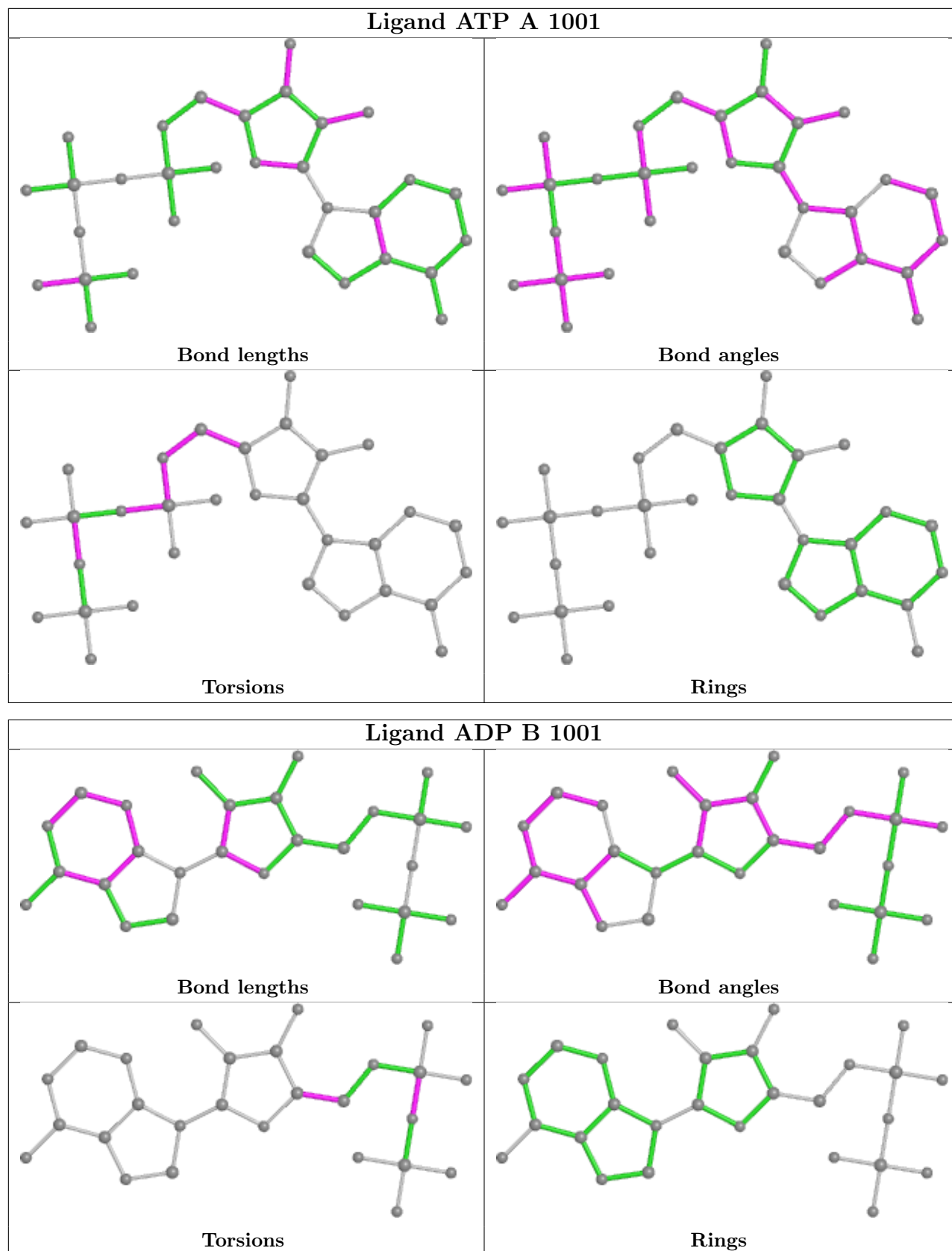
Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	C5'-O5'-PA-O2A
2	A	1001	ATP	C5'-O5'-PA-O3A
3	B	1001	ADP	C3'-C4'-C5'-O5'
3	B	1001	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	ADP	2	0
4	B	1	PGE	8	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.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	381/413 (92%)	0.03	19 (4%) 28 27	27, 51, 98, 148	0
1	B	381/413 (92%)	0.11	25 (6%) 18 17	33, 56, 111, 149	0
All	All	762/826 (92%)	0.07	44 (5%) 23 22	27, 53, 106, 149	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	622	GLN	4.6
1	B	662	ASN	4.6
1	A	647	ASN	4.3
1	B	805	PRO	4.3
1	B	623	TYR	4.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

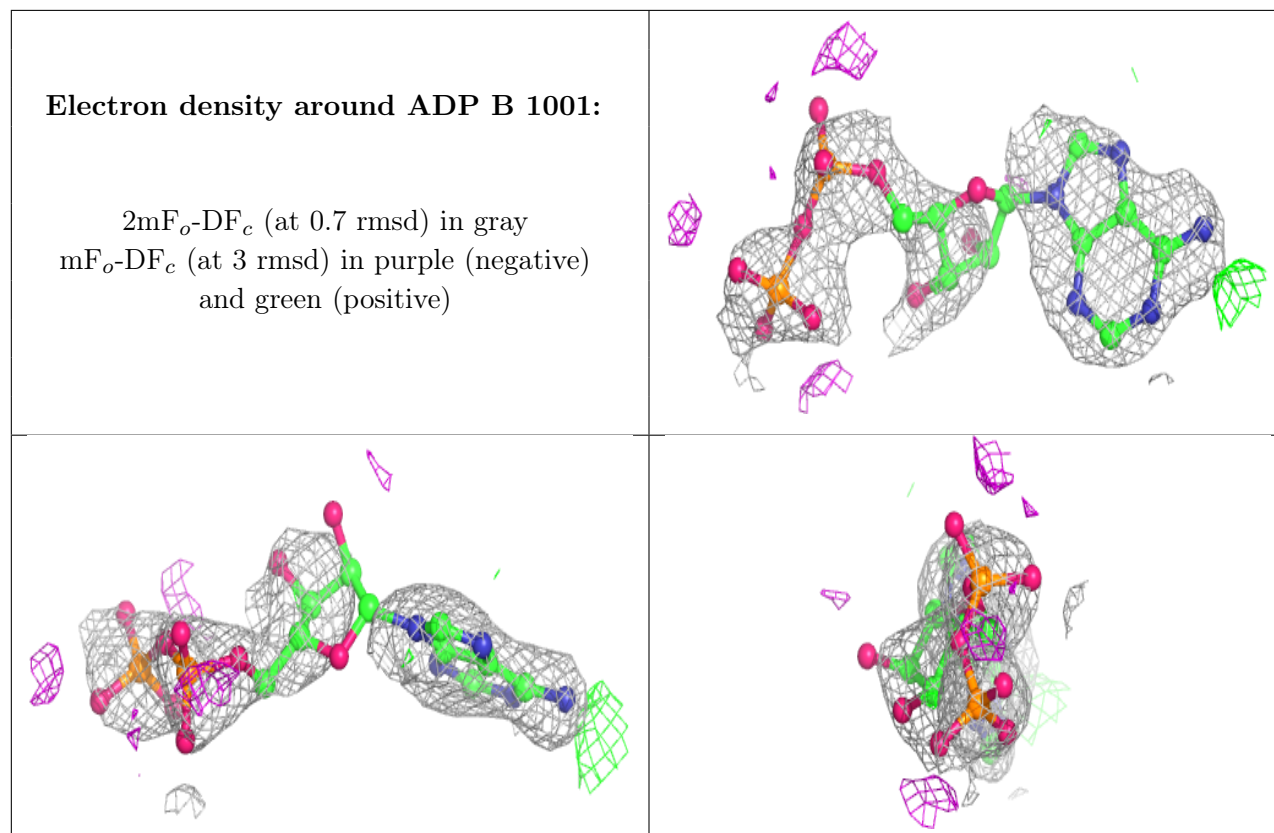
There are no monosaccharides in this entry.

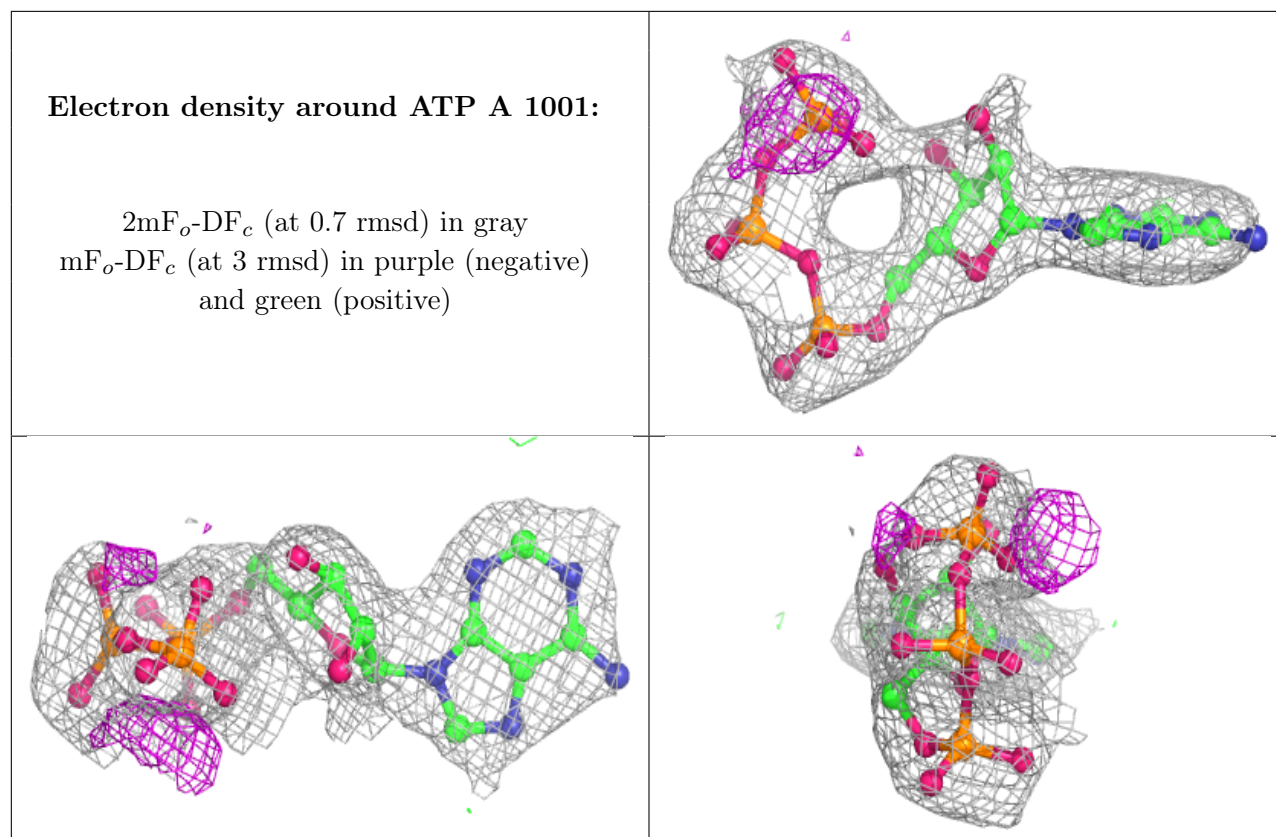
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	B	1001	27/27	0.81	0.41	91,137,167,252	0
4	PGE	B	1	10/10	0.90	0.22	55,63,69,70	0
2	ATP	A	1001	31/31	0.96	0.28	74,79,89,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.