



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 08:03 am BST

PDB ID : 3KX2  
Title : Crystal structure of Prp43p in complex with ADP  
Authors : Nielsen, K.H.; Andersen, G.R.; He, Y.  
Deposited on : 2009-12-02  
Resolution : 2.20 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.

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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	:	2.11
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)	:	2.11

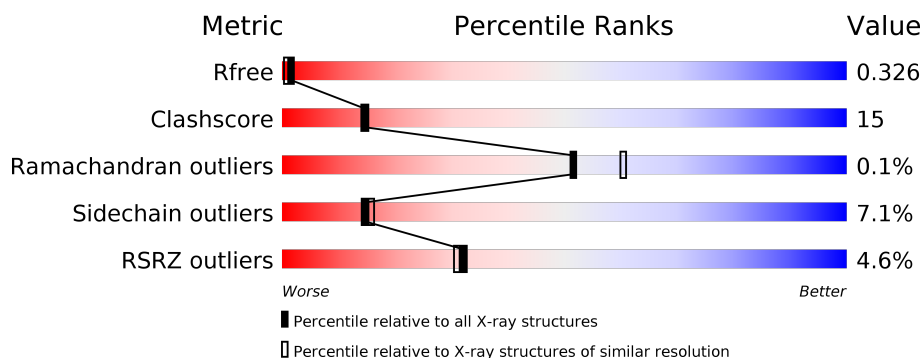
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	767	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	767	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>5% •</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13172 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.

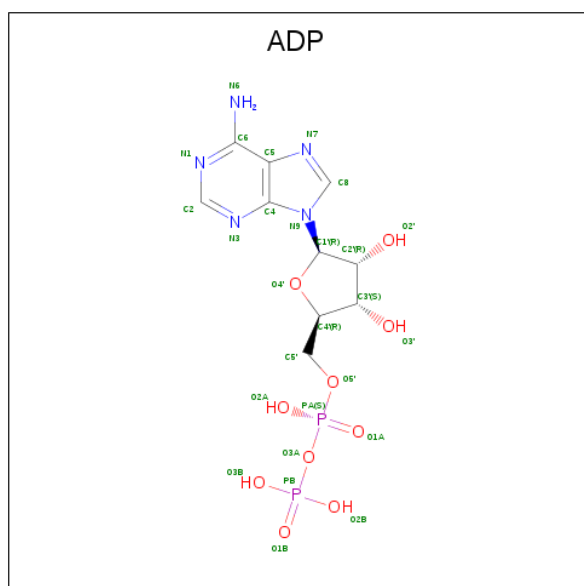
- Molecule 1 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	755	Total	C	N	O	S	0	0	0
			6067	3841	1048	1153	25			
1	A	755	Total	C	N	O	S	0	0	0
			6067	3841	1048	1153	25			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- 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
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	538	Total	O	0	0
			538	538		
4	A	444	Total	O	0	0
			444	444		

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

- Chain B:

73% 21% 5% 3%

Label	Value	Category
T711	1619	Green
R714	1608	Green
P715	1619	Green
E716	1620	Green
W717	1623	Green
P723	1624	Green
L728	1625	Green
S729	1626	Green
N730	1627	Green
F731	1628	Green
Q732	1629	Green
K733	1630	Green
W734	1631	Green
D735	1632	Green
V736	1633	Green
K737	1634	Green
L738	1635	Green
S739	1636	Green
L740	1637	Green
E741	1638	Green
R742	1639	Green
I743	1640	Green
E744	1641	Green
E745	1642	Green
W746	1643	Green
D747	1644	Green
L748	1645	Green
R749	1646	Green
L750	1647	Green
N751	1648	Green
E752	1649	Green
L753	1650	Green
K754	1651	Green
Q755	1652	Green
GLY	1653	Green
LYS	1654	Green
ASN	1655	Green
LYS	1656	Green
LYS	1657	Green
LYS	1658	Green
SER	1659	Green
LYS	1660	Green
LYS	1661	Green
HIS	1662	Green
SER	1663	Green
LYS	1664	Green
LYS	1665	Green
LYS	1666	Green
LYS	1667	Green
LYS	1668	Green
LYS	1669	Green
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LYS	1759	Green
LYS	1760	Green
LYS	1761	Green
LYS	1762	Green
LYS	1763	Green
LYS	1764	Green
LYS	1765	Green
LYS	1766	Green
LYS	1767	Green

- Chain A:
- 
- 6% 73% 21%
- M1 G2 R6 E10 H34 P35 L36 P37 V43 A47 G48 E49 L53 T58 S59 A60 E61 E62 A63 Q64 K65 L66 K70 I71 N72 P73 G76 R77 E78 P81 K82 Y83 V84 K88 I89 E92 L93 P94 Q110 V113 F114 V115 T118 G119
- D133 T146 P147 A148 R149 R150 V151 M154 S155 V156 M164 D165 V166 E170 Y174 S175 I176 R177 F178 E179 N180 S183 T186 Y190 M191 T192 D193 L197 L214 D215 T221 L222 A223 T224 L230 L231 D232 V235 R238 P239 D240 I243 L250 P251
- A252 E253 R257 Y258 L264 L265 T271 Q283 R284 S289 T293 Q296 I297 E298 E302 T311 E315 I316 E317 V320 S324 P338 L339 L344 L348 P349 P350 R351 Q352 Q353 Q354 R355 I356 G369 R370 R371 V372 T376 N377 I378 T381 P382



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.15Å 118.15Å 253.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.42 – 2.20 48.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.42-2.20) 99.8 (48.42-2.20)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.206 , 0.250 0.301 , 0.326	Depositor DCC
$R_{free}$ test set	5221 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.71	18/6195 (0.3%)	0.58	6/8384 (0.1%)
1	B	0.59	16/6195 (0.3%)	0.61	9/8384 (0.1%)
All	All	0.65	34/12390 (0.3%)	0.59	15/16768 (0.1%)

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	GLU	CD-OE2	-17.97	1.05	1.25
1	A	317	GLU	CD-OE1	-17.68	1.06	1.25
1	A	83	TYR	CE2-CZ	-17.41	1.16	1.38
1	B	83	TYR	CD1-CE1	-17.22	1.13	1.39
1	B	83	TYR	CD2-CE2	-15.92	1.15	1.39

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	734	GLY	N-CA-C	12.59	144.58	113.10
1	B	215	ASP	CB-CG-OD1	9.86	127.17	118.30
1	A	232	LYS	CB-CA-C	9.33	129.06	110.40
1	B	733	LYS	N-CA-C	8.59	134.18	111.00
1	A	215	ASP	CB-CG-OD1	8.56	126.01	118.30

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	6067	0	6035	184	0
1	B	6067	0	6035	185	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	3	0
4	A	444	0	0	14	0
4	B	538	0	0	19	0
All	All	13172	0	12094	374	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 15.

The worst 5 of 374 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:70:LYS:HE2	1:A:70:LYS:H	1.13	1.13
1:B:735:ASP:HB2	1:B:737:LYS:HE3	1.27	1.13
1:B:70:LYS:HE2	1:B:70:LYS:H	1.13	1.13
1:A:737:LYS:H	1:A:737:LYS:HE2	1.10	1.12
1:B:737:LYS:H	1:B:737:LYS:HE2	1.10	1.11

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	753/767 (98%)	723 (96%)	29 (4%)	1 (0%)	51	60
1	B	753/767 (98%)	722 (96%)	31 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1506/1534 (98%)	1445 (96%)	60 (4%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	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 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	668/679 (98%)	622 (93%)	46 (7%)	15 16
1	B	668/679 (98%)	619 (93%)	49 (7%)	14 15
All	All	1336/1358 (98%)	1241 (93%)	95 (7%)	14 16

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	707	ILE
1	A	70	LYS
1	A	699	PHE
1	B	735	ASP
1	B	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	647	ASN
1	A	54	GLN
1	A	647	ASN
1	B	659	GLN
1	B	730	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
3	ADP	B	1000	2	24,29,29	1.39	4 (16%)	29,45,45	1.39	3 (10%)
3	ADP	A	1000	2	24,29,29	1.38	4 (16%)	29,45,45	1.42	3 (10%)

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	ADP	B	1000	2	-	3/12/32/32	0/3/3/3
3	ADP	A	1000	2	-	3/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	ADP	O4'-C1'	3.99	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	ADP	O4'-C1'	3.94	1.46	1.41
3	A	1000	ADP	C5-C4	2.59	1.47	1.40
3	A	1000	ADP	C2-N3	2.52	1.36	1.32
3	B	1000	ADP	C5-C4	2.46	1.47	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	ADP	C3'-C2'-C1'	4.25	107.37	100.98
3	B	1000	ADP	C3'-C2'-C1'	4.10	107.16	100.98
3	A	1000	ADP	O5'-C5'-C4'	-2.91	98.97	108.99
3	B	1000	ADP	O5'-C5'-C4'	-2.85	99.19	108.99
3	A	1000	ADP	O4'-C1'-C2'	-2.31	103.55	106.93

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1000	ADP	O4'-C4'-C5'-O5'
3	A	1000	ADP	O4'-C4'-C5'-O5'
3	B	1000	ADP	C3'-C4'-C5'-O5'
3	A	1000	ADP	C3'-C4'-C5'-O5'
3	B	1000	ADP	C5'-O5'-PA-O2A

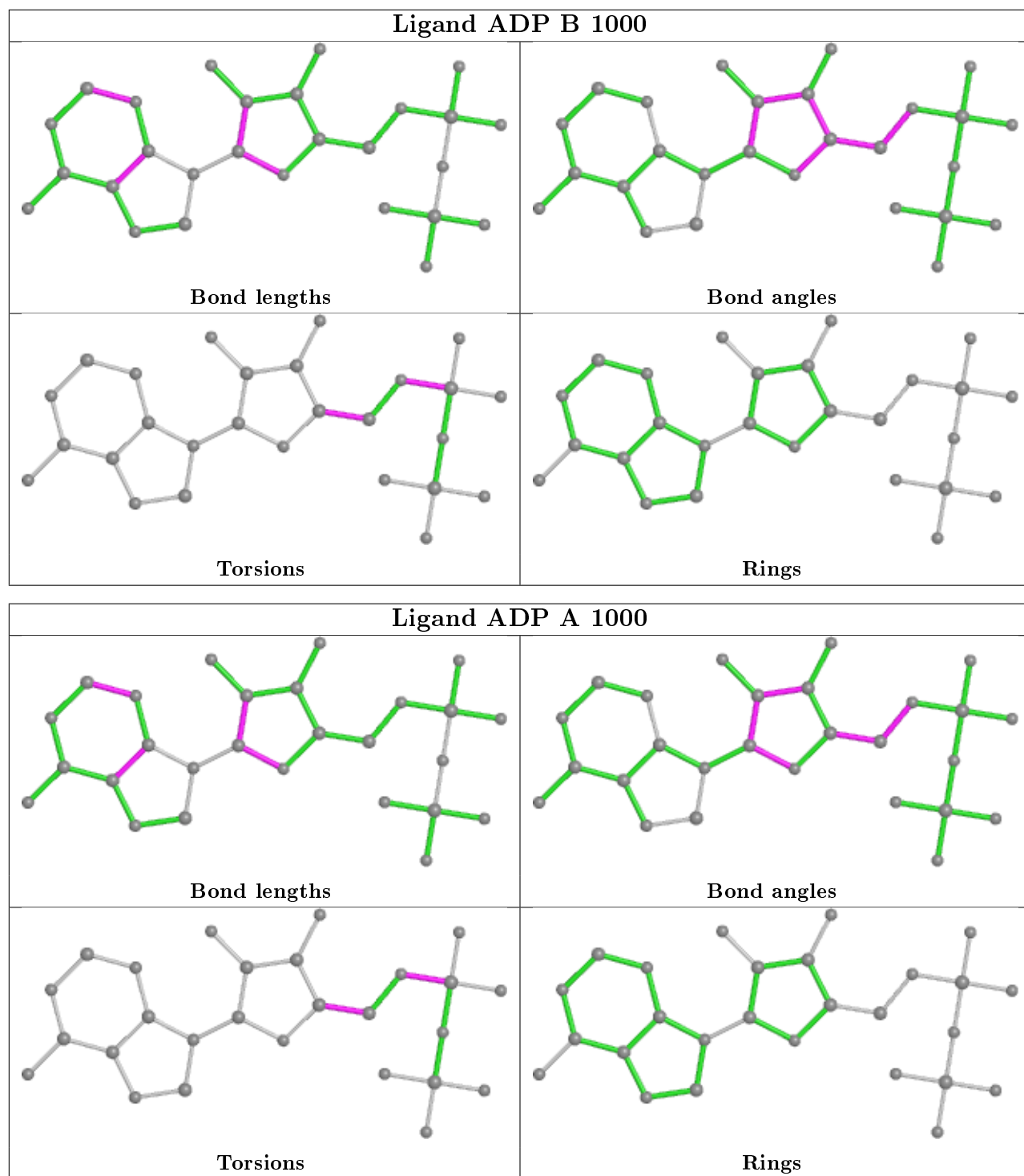
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	ADP	3	0
3	A	1000	ADP	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 ⓘ

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	755/767 (98%)	0.19	43 (5%)	23 22	23, 48, 100, 191	0
1	B	755/767 (98%)	0.02	26 (3%)	45 43	22, 44, 100, 191	0
All	All	1510/1534 (98%)	0.11	69 (4%)	32 31	22, 46, 100, 191	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	14.5
1	A	1	MET	13.5
1	B	755	GLN	9.7
1	B	754	LYS	9.6
1	A	754	LYS	8.3

### 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](#)

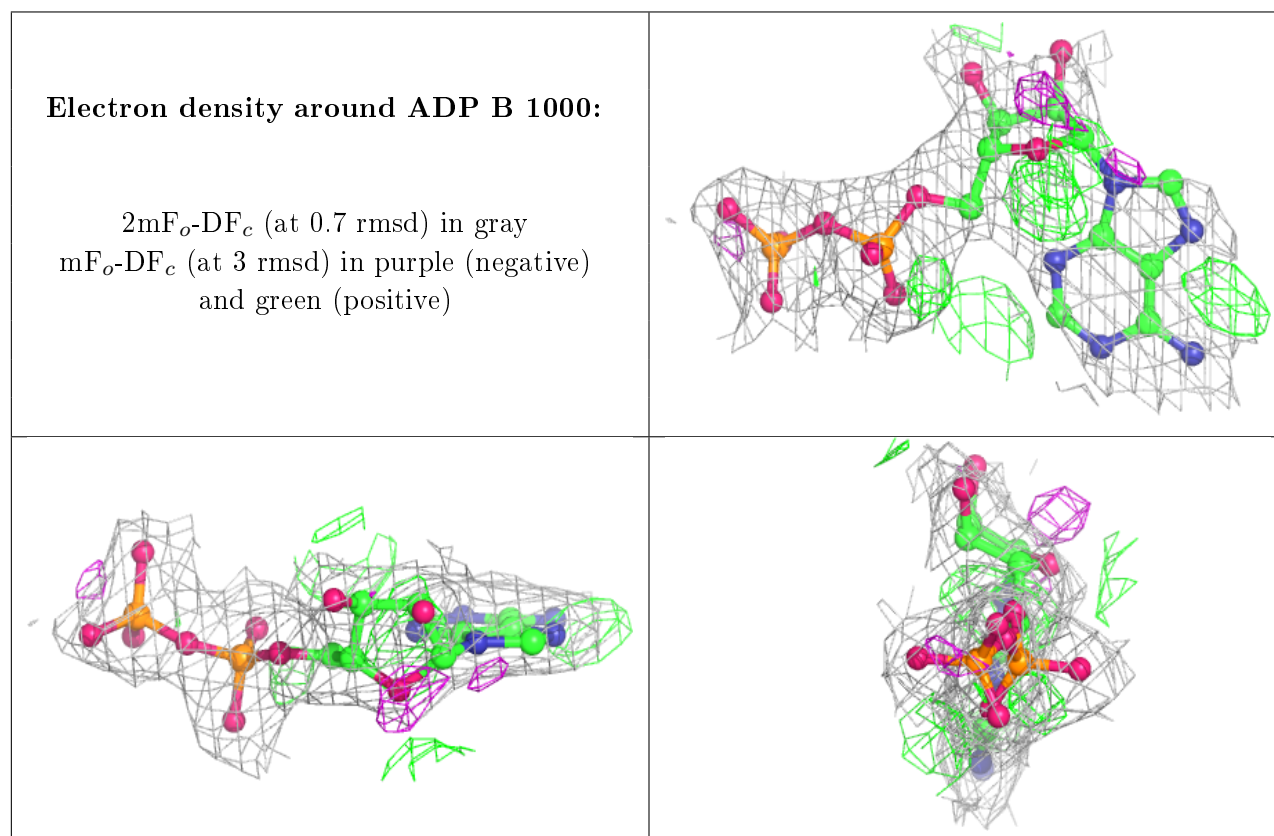
There are no carbohydrates in this entry.

### 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	1000	27/27	0.95	0.19	23,54,71,84	0
3	ADP	A	1000	27/27	0.95	0.16	26,50,70,83	0
2	MG	B	800	1/1	0.96	0.18	32,32,32,32	0
2	MG	A	800	1/1	0.98	0.19	31,31,31,31	0

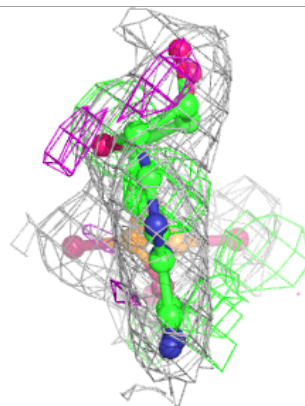
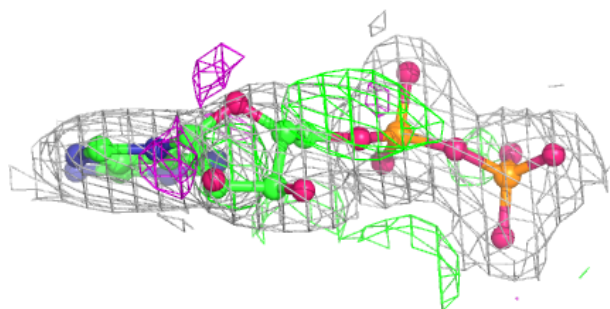
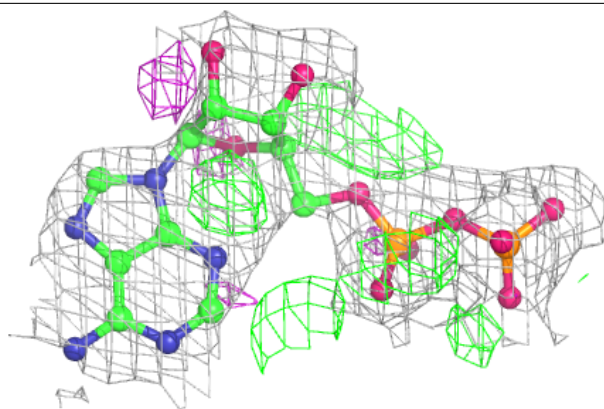
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





**Electron density around ADP A 1000:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.