



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:11 PM GMT

PDB ID : 1NY3  
Title : Crystal structure of ADP bound to MAP KAP kinase 2  
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Deposited on : 2003-02-11  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

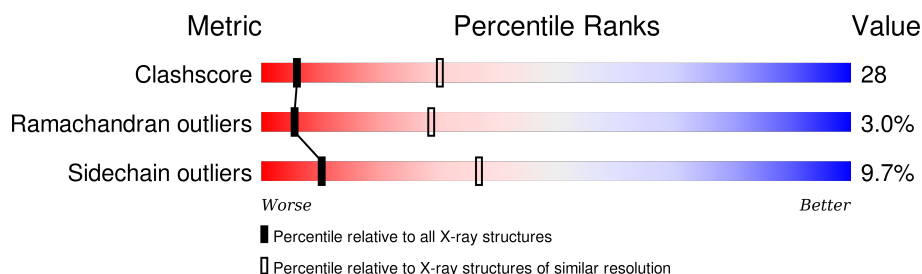
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	400	<div> <div></div> <div>35%</div> <div>29%</div> <div>5%</div> <div>31%</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2207 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2180	1396	368	399	17	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



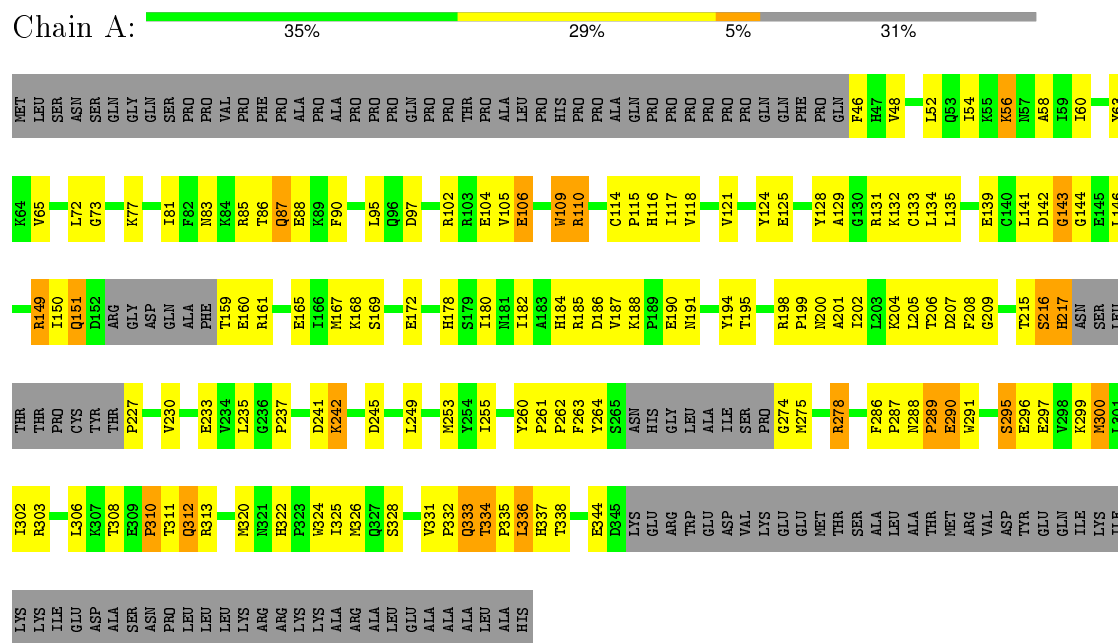
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: MAP kinase-activated protein kinase 2



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	253.05Å 253.05Å 253.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	93.9 (20.00-3.00)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.259 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

## 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: 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	0.49	1/2227 (0.0%)	0.73	1/3016 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	TRP	NE1-CE2	8.73	1.48	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	O-C-N	-5.36	114.13	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	217	HIS	Sidechain

## 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	2180	0	2142	124	0
2	A	27	0	12	3	0
All	All	2207	0	2154	124	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 28.

All (124) 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:102:ARG:NH2	1:A:125:GLU:HG3	1.74	1.00
1:A:328:SER:O	1:A:331:VAL:HG12	1.62	0.97
1:A:216:SER:CB	1:A:217:HIS:HA	1.97	0.93
1:A:216:SER:HB3	1:A:217:HIS:HA	1.54	0.87
1:A:190:GLU:CD	1:A:190:GLU:H	1.79	0.85
1:A:46:PHE:HE1	1:A:48:VAL:HG21	1.40	0.84
1:A:102:ARG:HH22	1:A:125:GLU:HG3	1.42	0.84
1:A:202:ILE:HD11	1:A:204:LYS:HE3	1.61	0.83
1:A:114:CYS:HB3	1:A:117:ILE:HD12	1.61	0.82
1:A:54:ILE:HD12	1:A:102:ARG:NH1	1.97	0.80
1:A:46:PHE:CE1	1:A:48:VAL:HG21	2.16	0.80
1:A:118:VAL:HB	1:A:206:THR:HG22	1.63	0.79
1:A:159:THR:HG22	1:A:333:GLN:O	1.87	0.75
1:A:115:PRO:O	1:A:204:LYS:HE2	1.88	0.74
1:A:275:MET:HA	1:A:278:ARG:HG3	1.71	0.71
1:A:161:ARG:HA	1:A:331:VAL:HG13	1.74	0.70
1:A:227:PRO:O	1:A:230:VAL:HG12	1.90	0.70
1:A:73:GLY:HA3	2:A:401:ADP:O3B	1.91	0.68
1:A:202:ILE:HD11	1:A:204:LYS:CE	2.23	0.68
1:A:161:ARG:HA	1:A:331:VAL:CG1	2.26	0.66
1:A:86:THR:HG22	1:A:88:GLU:HG2	1.78	0.66
1:A:52:LEU:HD23	1:A:106:GLU:OE1	1.95	0.65
1:A:260:TYR:OH	1:A:287:PRO:HG2	1.96	0.65
1:A:129:ALA:C	1:A:131:ARG:H	2.00	0.64
1:A:178:HIS:CE1	1:A:242:LYS:HB2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:CE1	1:A:48:VAL:CG2	2.81	0.64
1:A:90:PHE:CE2	1:A:121:VAL:HG21	2.32	0.64
1:A:161:ARG:O	1:A:165:GLU:HG3	1.97	0.64
1:A:58:ALA:HB1	1:A:60:ILE:HG12	1.80	0.62
1:A:149:ARG:HH11	1:A:149:ARG:HB3	1.63	0.62
1:A:168:LYS:O	1:A:172:GLU:HG3	2.00	0.61
1:A:274:GLY:O	1:A:278:ARG:HG2	2.01	0.60
1:A:198:ARG:CG	1:A:199:PRO:HD2	2.32	0.60
1:A:83:ASN:O	1:A:87:GLN:N	2.31	0.59
1:A:54:ILE:CG2	1:A:125:GLU:HB2	2.34	0.58
1:A:54:ILE:HD12	1:A:102:ARG:HH11	1.66	0.58
1:A:216:SER:HB3	1:A:217:HIS:CA	2.31	0.57
1:A:242:LYS:O	1:A:245:ASP:HB2	2.04	0.57
1:A:63:TYR:HE2	1:A:124:TYR:HH	1.51	0.57
1:A:72:LEU:HD23	1:A:77:LYS:HA	1.85	0.57
1:A:206:THR:O	1:A:207:ASP:HB3	2.05	0.56
1:A:206:THR:O	1:A:207:ASP:CB	2.53	0.56
1:A:141:LEU:O	2:A:401:ADP:H2	1.87	0.56
1:A:118:VAL:CB	1:A:206:THR:HG22	2.35	0.56
1:A:198:ARG:HG2	1:A:199:PRO:HD2	1.88	0.56
1:A:128:TYR:HB3	1:A:133:CYS:SG	2.46	0.56
1:A:161:ARG:CA	1:A:331:VAL:HG13	2.37	0.55
1:A:216:SER:CB	1:A:217:HIS:CA	2.78	0.54
1:A:300:MET:CE	1:A:303:ARG:HD2	2.37	0.54
1:A:188:LYS:HB2	1:A:190:GLU:OE1	2.07	0.54
1:A:160:GLU:HB2	1:A:334:THR:HG23	1.91	0.53
1:A:129:ALA:C	1:A:131:ARG:N	2.62	0.52
1:A:288:ASN:C	1:A:290:GLU:OE1	2.47	0.52
1:A:141:LEU:O	2:A:401:ADP:C2	2.63	0.52
1:A:325:ILE:HG22	1:A:326:MET:N	2.24	0.52
1:A:116:HIS:CE1	1:A:169:SER:HB2	2.46	0.51
1:A:161:ARG:HB2	1:A:331:VAL:O	2.11	0.51
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.93	0.51
1:A:65:VAL:HA	1:A:81:ILE:HG22	1.93	0.50
1:A:149:ARG:HG3	1:A:194:TYR:CD2	2.47	0.50
1:A:167:MET:HG3	1:A:253:MET:HG3	1.93	0.50
1:A:161:ARG:CB	1:A:331:VAL:HG13	2.43	0.49
1:A:105:VAL:HG21	1:A:134:LEU:HD23	1.94	0.49
1:A:172:GLU:HG2	1:A:320:MET:CE	2.42	0.49
1:A:290:GLU:N	1:A:290:GLU:OE1	2.45	0.49
1:A:195:THR:CG2	1:A:202:ILE:HG12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:HIS:NE2	1:A:242:LYS:CB	2.76	0.49
1:A:178:HIS:NE2	1:A:242:LYS:HB2	2.28	0.49
1:A:320:MET:HA	1:A:325:ILE:HG21	1.95	0.48
1:A:184:HIS:CE1	1:A:207:ASP:O	2.67	0.48
1:A:160:GLU:CB	1:A:334:THR:HG23	2.44	0.48
1:A:190:GLU:CD	1:A:190:GLU:N	2.59	0.47
1:A:54:ILE:CD1	1:A:102:ARG:NH1	2.73	0.47
1:A:118:VAL:CG1	1:A:206:THR:HG22	2.44	0.47
1:A:278:ARG:HH11	1:A:278:ARG:HG3	1.80	0.47
1:A:52:LEU:HB2	1:A:109:TRP:CD1	2.48	0.47
1:A:142:ASP:O	1:A:144:GLY:N	2.48	0.47
1:A:195:THR:HG21	1:A:202:ILE:HG12	1.97	0.47
1:A:104:GLU:OE1	1:A:209:GLY:HA2	2.15	0.47
1:A:255:ILE:HG12	1:A:261:PRO:HA	1.96	0.46
1:A:286:PHE:HB3	1:A:291:TRP:CG	2.51	0.46
1:A:237:PRO:HG2	1:A:237:PRO:O	2.16	0.46
1:A:310:PRO:O	1:A:313:ARG:N	2.43	0.46
1:A:310:PRO:O	1:A:312:GLN:N	2.50	0.45
1:A:180:ILE:HG13	1:A:182:ILE:HG13	1.98	0.45
1:A:333:GLN:HB3	1:A:333:GLN:HE21	1.48	0.45
1:A:160:GLU:HA	1:A:336:LEU:HD21	1.99	0.45
1:A:278:ARG:NH1	1:A:278:ARG:HG3	2.31	0.45
1:A:332:PRO:CB	1:A:334:THR:HG22	2.47	0.45
1:A:124:TYR:HB2	1:A:135:LEU:HB2	1.98	0.44
1:A:104:GLU:HG3	1:A:208:PHE:O	2.17	0.44
1:A:146:LEU:O	1:A:150:ILE:HD13	2.18	0.44
1:A:187:VAL:O	1:A:187:VAL:HG12	2.16	0.44
1:A:302:ILE:HG22	1:A:306:LEU:HD12	1.99	0.44
1:A:184:HIS:ND1	1:A:205:LEU:HD21	2.33	0.43
1:A:180:ILE:HD11	1:A:182:ILE:HD12	2.01	0.43
1:A:331:VAL:HG23	1:A:332:PRO:HD2	2.01	0.42
1:A:118:VAL:HB	1:A:206:THR:CG2	2.43	0.42
1:A:150:ILE:HG22	1:A:151:GLN:N	2.34	0.42
1:A:97:ASP:OD2	1:A:132:LYS:HE2	2.20	0.42
1:A:143:GLY:HA3	1:A:194:TYR:CB	2.49	0.42
1:A:322:HIS:CE1	1:A:324:TRP:HB2	2.55	0.42
1:A:275:MET:HA	1:A:278:ARG:HH11	1.84	0.42
1:A:331:VAL:CG2	1:A:332:PRO:HD2	2.49	0.42
1:A:129:ALA:O	1:A:131:ARG:N	2.53	0.42
1:A:143:GLY:N	1:A:194:TYR:O	2.52	0.42
1:A:167:MET:CE	1:A:249:LEU:HG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:TYR:OH	1:A:287:PRO:CG	2.65	0.42
1:A:289:PRO:HG2	1:A:290:GLU:H	1.85	0.42
1:A:118:VAL:HG23	1:A:139:GLU:HG2	2.01	0.41
1:A:296:GLU:O	1:A:300:MET:HB2	2.20	0.41
1:A:278:ARG:HG2	1:A:278:ARG:H	1.42	0.41
1:A:295:SER:OG	1:A:297:GLU:HB3	2.20	0.41
1:A:296:GLU:HA	1:A:299:LYS:HB2	2.03	0.41
1:A:161:ARG:HA	1:A:331:VAL:HG11	2.02	0.41
1:A:185:ARG:HD2	1:A:185:ARG:HH11	1.63	0.41
1:A:289:PRO:O	1:A:291:TRP:N	2.54	0.41
1:A:335:PRO:O	1:A:336:LEU:HD13	2.22	0.40
1:A:200:ASN:O	1:A:201:ALA:C	2.58	0.40
1:A:188:LYS:HE2	1:A:191:ASN:OD1	2.22	0.40
1:A:190:GLU:N	1:A:190:GLU:OE1	2.47	0.40
1:A:172:GLU:HG2	1:A:320:MET:HE2	2.02	0.40
1:A:262:PRO:HG2	1:A:263:PHE:H	1.86	0.40
1:A:56:LYS:HE2	1:A:125:GLU:OE1	2.21	0.40

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	269/400 (67%)	228 (85%)	33 (12%)	8 (3%)	<b>5</b> <b>29</b>

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	GLU
1	A	143	GLY
1	A	241	ASP
1	A	311	THR

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Mol	Chain	Res	Type
1	A	338	THR
1	A	186	ASP
1	A	310	PRO
1	A	289	PRO

### 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	236/357 (66%)	213 (90%)	23 (10%)	10	37

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	85	ARG
1	A	87	GLN
1	A	106	GLU
1	A	110	ARG
1	A	149	ARG
1	A	151	GLN
1	A	215	THR
1	A	216	SER
1	A	233	GLU
1	A	235	LEU
1	A	242	LYS
1	A	264	TYR
1	A	278	ARG
1	A	295	SER
1	A	300	MET
1	A	308	THR
1	A	312	GLN
1	A	333	GLN
1	A	334	THR
1	A	336	LEU
1	A	337	HIS

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Mol	Chain	Res	Type
1	A	344	GLU

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

Mol	Chain	Res	Type
1	A	53	GLN
1	A	68	GLN
1	A	87	GLN
1	A	113	GLN
1	A	151	GLN
1	A	184	HIS
1	A	304	ASN
1	A	333	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 carbohydrates 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
2	ADP	A	401	-	22,29,29	1.31	2 (9%)	27,45,45	2.71	3 (11%)

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	ADP	A	401	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ADP	C5-N7	-2.41	1.31	1.39
2	A	401	ADP	O4'-C1'	3.36	1.45	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ADP	N3-C2-N1	-13.14	118.83	128.89
2	A	401	ADP	C4-C5-N7	-2.29	107.37	109.48
2	A	401	ADP	O3A-PA-O5'	2.07	108.43	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ADP	3	0

## 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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.