



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:57 pm GMT

PDB ID : 1Q0B  
Title : Crystal structure of the motor protein KSP in complex with ADP and monastrol  
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Deposited on : 2003-07-15  
Resolution : 1.90 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

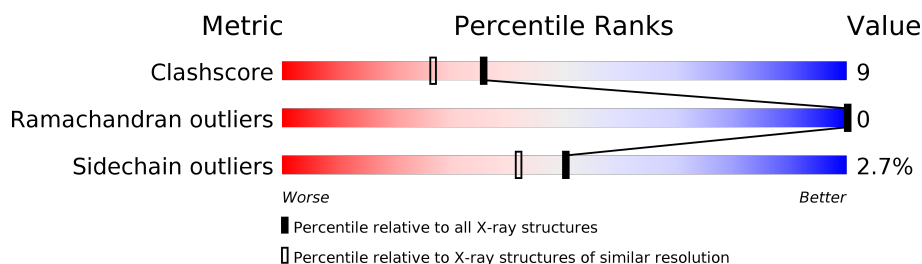
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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	367	 72% 17% 10%
1	B	367	 72% 19% 9%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5825 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 Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2599	1628	453	508	10			
1	B	335	Total	C	N	O	S	0	0	0
			2630	1647	458	515	10			

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

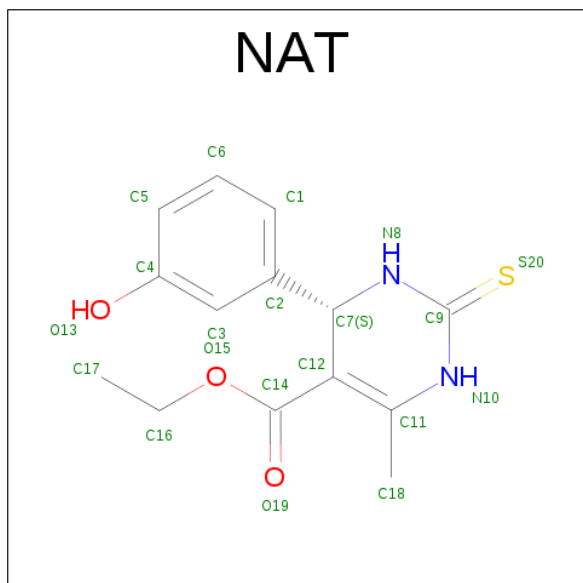
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

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

- Molecule 4 is ETHYL 4-(3-HYDROXYPHENYL)-6-METHYL-2-THIOXO-1,2,3,4-TETRAHYDOPYRIMIDINE-5-CARBOXYLATE (three-letter code: NAT) (formula:  $C_{14}H_{16}N_2O_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	14	2	3	1		
4	B	1	Total	C	N	O	S	0	0
			20	14	2	3	1		

- Molecule 5 is water.

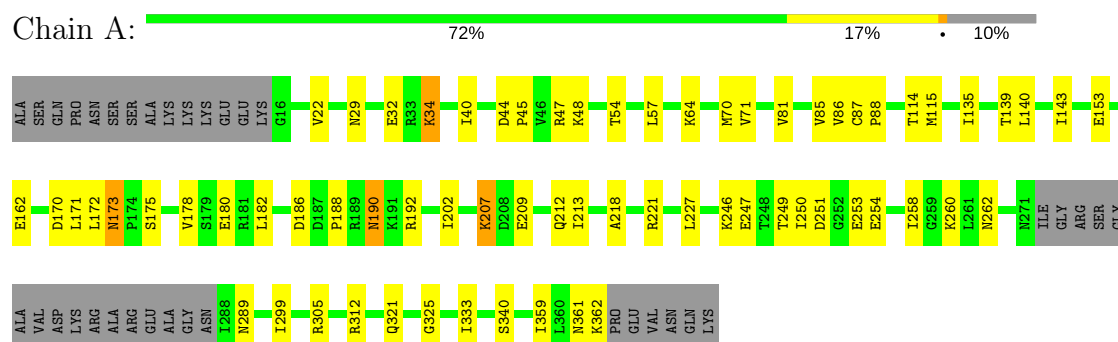
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total	O	0	0
			250	250		
5	B	250	Total	O	0	0
			250	250		

### 3 Residue-property plots

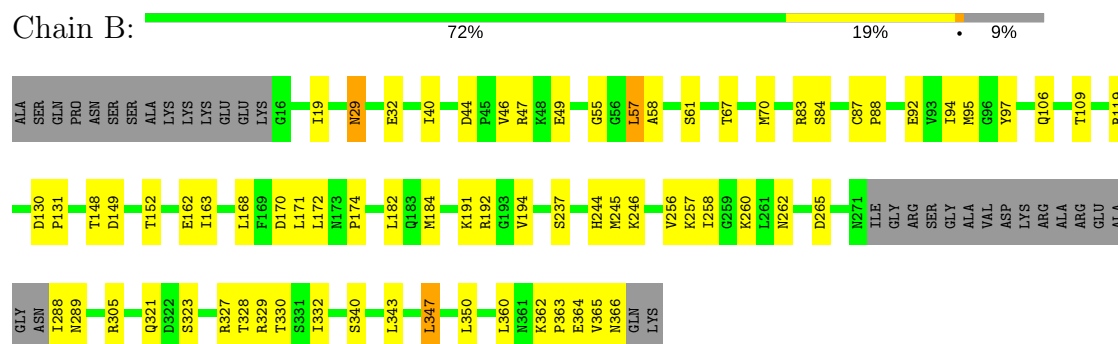
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: Kinesin-like protein KIF11



#### • Molecule 1: Kinesin-like protein KIF11



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.30Å 79.50Å 159.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	99.0 (20.00-1.90)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.219 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5825	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAT, 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	0.30	0/2637	0.59	0/3564
1	B	0.30	0/2669	0.60	0/3609
All	All	0.30	0/5306	0.59	0/7173

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	2599	0	2627	46	0
1	B	2630	0	2655	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	20	0	15	2	0
4	B	20	0	15	2	0
5	A	250	0	0	3	0
5	B	250	0	0	1	0
All	All	5825	0	5336	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 9.

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:B:162:GLU:HG3	1:B:171:LEU:HD13	1.42	0.97
1:B:49:GLU:HG2	1:B:67:THR:HG22	1.52	0.89
1:A:81:VAL:O	1:A:85:VAL:HG12	1.77	0.84
1:A:45:PRO:HA	1:A:71:VAL:HG13	1.61	0.82
1:B:92:GLU:HG3	1:B:329:ARG:NH1	1.99	0.78
1:B:327:ARG:HD3	1:B:364:GLU:OE2	1.83	0.77
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.67	0.76
1:A:115:MET:HE1	1:A:135:ILE:HD12	1.68	0.74
1:B:162:GLU:HG3	1:B:171:LEU:CD1	2.18	0.73
1:A:48:LYS:HA	1:A:71:VAL:HG12	1.72	0.71
1:B:246:LYS:HG2	1:B:256:VAL:HG12	1.76	0.67
4:A:604:NAT:H181	4:A:604:NAT:O15	1.95	0.66
1:A:325:GLY:H	1:A:361:ASN:HD21	1.44	0.65
1:A:207:LYS:NZ	1:A:207:LYS:HB3	2.12	0.64
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.80	0.64
1:A:173:ASN:ND2	1:A:175:SER:H	1.95	0.63
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.78	0.63
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.80	0.63
1:A:45:PRO:HA	1:A:71:VAL:CG1	2.28	0.63
1:A:87:CYS:HB3	1:A:88:PRO:HD3	1.81	0.63
1:A:209:GLU:HA	1:A:212:GLN:HE21	1.64	0.63
1:B:40:ILE:HD13	1:B:340:SER:HA	1.80	0.63
1:A:22:VAL:HG12	1:A:70:MET:HB2	1.82	0.61
1:A:162:GLU:HG3	1:A:171:LEU:HD23	1.83	0.61
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.67	0.60
1:A:178:VAL:HG23	1:A:227:LEU:HD12	1.84	0.59
1:B:29:ASN:ND2	1:B:32:GLU:H	2.01	0.58
1:A:207:LYS:HB3	1:A:207:LYS:HZ3	1.67	0.58
1:B:57:LEU:O	1:B:61:SER:HB3	2.04	0.58
1:B:172:LEU:O	1:B:174:PRO:HD3	2.05	0.57
1:B:92:GLU:HG3	1:B:329:ARG:HH11	1.68	0.57
1:B:97:TYR:CZ	1:B:365:VAL:HG23	2.41	0.56
1:B:257:LYS:HG2	5:B:777:HOH:O	2.06	0.55
1:B:191:LYS:HG2	1:B:192:ARG:NH1	2.22	0.54
1:B:19:ILE:HD11	1:B:332:ILE:HG13	1.89	0.54
1:B:97:TYR:CE1	1:B:365:VAL:HG23	2.42	0.54
1:B:260:LYS:HE2	1:B:262:ASN:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:NZ	1:A:34:LYS:HB2	2.23	0.54
1:A:44:ASP:OD2	1:A:47:ARG:HD3	2.09	0.53
1:B:29:ASN:HD22	1:B:29:ASN:C	2.11	0.53
1:B:305:ARG:HH22	1:B:360:LEU:HD22	1.74	0.53
1:B:55:GLY:O	1:B:61:SER:HB2	2.09	0.53
1:A:114:THR:HG22	1:A:115:MET:HE2	1.90	0.52
1:A:190:ASN:OD1	1:A:190:ASN:N	2.42	0.52
1:A:325:GLY:H	1:A:361:ASN:ND2	2.07	0.52
1:A:40:ILE:HD13	1:A:340:SER:HA	1.92	0.51
1:B:29:ASN:HD22	1:B:32:GLU:H	1.58	0.51
1:B:29:ASN:HD21	1:B:32:GLU:HG3	1.75	0.51
1:B:94:ILE:HG23	1:B:245:MET:HE3	1.92	0.51
1:A:186:ASP:CG	1:A:312:ARG:HH22	2.15	0.51
1:A:172:LEU:HB3	1:A:202:ILE:CD1	2.43	0.49
1:B:184:MET:HE3	1:B:194:VAL:HG21	1.95	0.48
1:A:29:ASN:OD1	1:A:32:GLU:HG3	2.13	0.48
4:B:605:NAT:O15	4:B:605:NAT:H181	2.13	0.48
1:A:321:GLN:NE2	5:A:790:HOH:O	2.45	0.48
1:A:249:THR:HB	1:A:253:GLU:OE1	2.13	0.48
1:B:305:ARG:HH22	1:B:360:LEU:CD2	2.27	0.47
1:B:305:ARG:NH2	1:B:360:LEU:HD22	2.29	0.47
1:A:173:ASN:C	1:A:173:ASN:HD22	2.18	0.47
1:A:249:THR:HG22	1:A:250:ILE:N	2.29	0.47
1:B:119:ARG:HG2	4:B:605:NAT:H161	1.97	0.47
1:A:251:ASP:HB2	1:A:253:GLU:OE1	2.14	0.46
1:A:258:ILE:HD12	1:A:258:ILE:N	2.29	0.46
1:B:343:LEU:CD2	1:B:347:LEU:HD22	2.46	0.46
1:B:152:THR:HG21	1:B:245:MET:CE	2.46	0.45
1:B:148:THR:HG23	1:B:149:ASP:N	2.32	0.45
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.98	0.44
1:B:70:MET:CE	1:B:84:SER:HB3	2.47	0.44
1:B:152:THR:HG21	1:B:245:MET:HE2	1.99	0.44
1:B:365:VAL:CG1	1:B:366:ASN:N	2.80	0.44
1:A:153:GLU:HB3	1:A:246:LYS:HB3	2.00	0.44
1:B:130:ASP:HA	1:B:131:PRO:HD3	1.87	0.44
1:A:85:VAL:HG13	1:A:86:VAL:N	2.33	0.44
1:B:106:GLN:HG3	1:B:109:THR:HG23	1.99	0.44
1:A:247:GLU:O	1:A:254:GLU:HA	2.17	0.44
1:B:244:HIS:ND1	1:B:258:ILE:HG12	2.33	0.44
1:B:237:SER:HB3	1:B:265:ASP:HB3	2.00	0.43
1:A:186:ASP:O	1:A:188:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:O	1:B:363:PRO:HA	2.18	0.43
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.82	0.43
1:B:44:ASP:OD2	1:B:46:VAL:HG22	2.18	0.43
1:B:163:ILE:HG12	1:B:168:LEU:CD2	2.49	0.42
1:A:172:LEU:HB3	1:A:202:ILE:HD11	2.00	0.42
1:A:209:GLU:O	1:A:213:ILE:HG13	2.19	0.42
1:A:221:ARG:HD3	5:A:830:HOH:O	2.18	0.42
1:B:92:GLU:HA	1:B:95:MET:HE3	2.01	0.42
1:A:361:ASN:C	1:A:362:LYS:HG3	2.40	0.42
1:A:48:LYS:HA	1:A:71:VAL:CG1	2.45	0.42
1:A:180:GLU:HG2	5:A:812:HOH:O	2.19	0.42
1:A:22:VAL:CG2	1:A:333:ILE:HG12	2.48	0.42
1:A:218:ALA:HB2	4:A:604:NAT:H182	2.02	0.41
1:B:46:VAL:HG23	1:B:47:ARG:N	2.34	0.41
1:B:19:ILE:HG13	1:B:330:THR:O	2.21	0.41
1:B:94:ILE:HG23	1:B:245:MET:CE	2.50	0.41
1:B:57:LEU:CD2	1:B:58:ALA:H	2.34	0.41
1:B:192:ARG:HE	1:B:321:GLN:HE22	1.69	0.41
1:A:139:THR:O	1:A:143:ILE:HG13	2.21	0.40
1:B:323:SER:HA	1:B:328:THR:HB	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 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	327/367 (89%)	320 (98%)	7 (2%)	0	100	100
1	B	331/367 (90%)	325 (98%)	6 (2%)	0	100	100
All	All	658/734 (90%)	645 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	293/321 (91%)	284 (97%)	9 (3%)	45	36
1	B	297/321 (92%)	290 (98%)	7 (2%)	54	47
All	All	590/642 (92%)	574 (97%)	16 (3%)	50	42

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	57	LEU
1	A	140	LEU
1	A	173	ASN
1	A	190	ASN
1	A	192	ARG
1	A	207	LYS
1	A	289	ASN
1	A	305	ARG
1	B	29	ASN
1	B	57	LEU
1	B	288	ILE
1	B	289	ASN
1	B	347	LEU
1	B	350	LEU
1	B	362	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	212	GLN
1	A	229	ASN
1	A	244	HIS
1	A	262	ASN
1	A	289	ASN

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Mol	Chain	Res	Type
1	A	308	HIS
1	A	321	GLN
1	A	361	ASN
1	B	29	ASN
1	B	98	ASN
1	B	141	HIS
1	B	262	ASN
1	B	271	ASN
1	B	289	ASN
1	B	290	GLN

### 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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	A	601	2	25,29,29	1.47	4 (16%)	24,45,45	2.75	2 (8%)
4	NAT	A	604	-	21,21,21	2.61	9 (42%)	29,29,29	2.25	10 (34%)
3	ADP	B	600	2	25,29,29	1.52	5 (20%)	24,45,45	2.72	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAT	B	605	-	21,21,21	2.63	9 (42%)	29,29,29	2.34	9 (31%)

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	A	601	2	-	0/12/32/32	0/3/3/3
4	NAT	A	604	-	-	0/11/27/27	0/2/2/2
3	ADP	B	600	2	-	0/12/32/32	0/3/3/3
4	NAT	B	605	-	-	0/11/27/27	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	ADP	C5-N7	-2.49	1.31	1.39
3	B	600	ADP	PB-O3A	-2.46	1.56	1.60
3	A	601	ADP	C5-N7	-2.46	1.31	1.39
4	B	605	NAT	C2-C7	-2.31	1.48	1.52
4	A	604	NAT	C2-C7	-2.28	1.49	1.52
3	B	600	ADP	C5'-C4'	2.13	1.58	1.51
3	A	601	ADP	C5'-C4'	2.16	1.58	1.51
4	B	605	NAT	C9-N8	2.16	1.35	1.33
4	A	604	NAT	C9-N8	2.39	1.35	1.33
3	A	601	ADP	O4'-C1'	2.53	1.44	1.41
4	B	605	NAT	C5-C4	2.75	1.44	1.38
3	B	600	ADP	O4'-C1'	2.81	1.45	1.41
3	A	601	ADP	C2-N3	2.89	1.37	1.32
3	B	600	ADP	C2-N3	2.89	1.37	1.32
4	B	605	NAT	C6-C5	3.09	1.44	1.38
4	A	604	NAT	C5-C4	3.10	1.45	1.38
4	B	605	NAT	C3-C2	3.23	1.44	1.39
4	A	604	NAT	C3-C2	3.29	1.44	1.39
4	A	604	NAT	C6-C5	3.51	1.45	1.38
4	A	604	NAT	C6-C1	3.51	1.45	1.38
4	B	605	NAT	C6-C1	3.87	1.46	1.38
4	B	605	NAT	C1-C2	4.38	1.46	1.39
4	A	604	NAT	C3-C4	4.48	1.46	1.39
4	A	604	NAT	C1-C2	4.58	1.46	1.39
4	B	605	NAT	C3-C4	4.99	1.46	1.39
4	B	605	NAT	C11-N10	6.05	1.46	1.38

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	NAT	C11-N10	6.06	1.46	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ADP	N3-C2-N1	-12.41	118.05	128.86
3	B	600	ADP	N3-C2-N1	-12.34	118.11	128.86
4	B	605	NAT	C4-C3-C2	-3.30	117.20	120.06
4	B	605	NAT	O19-C14-C12	-3.22	118.53	125.21
4	A	604	NAT	C9-N10-C11	-3.14	121.93	123.83
4	A	604	NAT	C4-C3-C2	-2.93	117.52	120.06
4	A	604	NAT	C5-C6-C1	-2.61	116.57	120.24
4	A	604	NAT	O19-C14-C12	-2.57	119.87	125.21
4	B	605	NAT	C5-C6-C1	-2.48	116.75	120.24
4	A	604	NAT	S20-C9-N10	-2.23	119.20	122.06
4	B	605	NAT	C9-N10-C11	-2.08	122.58	123.83
4	B	605	NAT	C1-C2-C3	2.07	121.20	118.79
4	A	604	NAT	C1-C2-C3	2.10	121.23	118.79
3	B	600	ADP	C4'-O4'-C1'	2.23	112.14	109.77
3	A	601	ADP	C4'-O4'-C1'	2.35	112.27	109.77
4	A	604	NAT	O15-C14-C12	2.92	117.50	112.31
4	B	605	NAT	N10-C9-N8	3.86	118.99	116.19
4	A	604	NAT	N10-C9-N8	3.89	119.01	116.19
4	B	605	NAT	O15-C14-C12	4.45	120.19	112.31
4	A	604	NAT	C12-C7-N8	5.24	113.31	109.13
4	B	605	NAT	C12-C7-N8	5.63	113.62	109.13
4	B	605	NAT	C16-O15-C14	5.81	126.52	116.53
4	A	604	NAT	C16-O15-C14	6.32	127.39	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	NAT	2	0
4	B	605	NAT	2	0

## 5.7 Other polymers

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.