



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 07:02 AM GMT

PDB ID : 3CR7  
Title : Crystal structure of N-terminal truncation of APS Kinase from *Penicillium chrysogenum*: Ternary structure with ADP and PAPS  
Authors : Gay, S.C.; Segel, I.H.; Fisher, A.J.  
Deposited on : 2008-04-04  
Resolution : 2.50 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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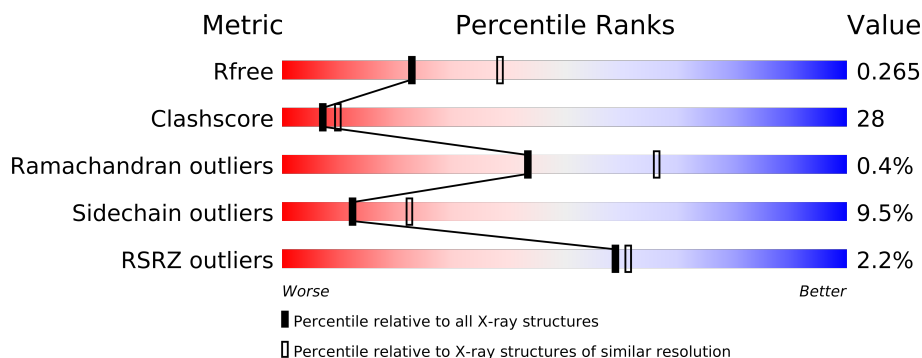
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	197	
1	B	197	
1	C	197	
1	D	197	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6230 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Adenylyl-sulfate kinase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	0	0	0
			1388	882	243	263			
1	B	181	Total	C	N	O	0	0	0
			1407	889	249	269			
1	C	178	Total	C	N	O	0	1	0
			1370	869	236	265			
1	D	183	Total	C	N	O	0	1	0
			1397	883	243	271			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	LEU	-	EXPRESSION TAG	UNP Q12657
A	213	GLU	-	EXPRESSION TAG	UNP Q12657
A	214	HIS	-	EXPRESSION TAG	UNP Q12657
A	215	HIS	-	EXPRESSION TAG	UNP Q12657
A	216	HIS	-	EXPRESSION TAG	UNP Q12657
A	217	HIS	-	EXPRESSION TAG	UNP Q12657
A	218	HIS	-	EXPRESSION TAG	UNP Q12657
A	219	HIS	-	EXPRESSION TAG	UNP Q12657
B	212	LEU	-	EXPRESSION TAG	UNP Q12657
B	213	GLU	-	EXPRESSION TAG	UNP Q12657
B	214	HIS	-	EXPRESSION TAG	UNP Q12657
B	215	HIS	-	EXPRESSION TAG	UNP Q12657
B	216	HIS	-	EXPRESSION TAG	UNP Q12657
B	217	HIS	-	EXPRESSION TAG	UNP Q12657
B	218	HIS	-	EXPRESSION TAG	UNP Q12657
B	219	HIS	-	EXPRESSION TAG	UNP Q12657
C	212	LEU	-	EXPRESSION TAG	UNP Q12657
C	213	GLU	-	EXPRESSION TAG	UNP Q12657
C	214	HIS	-	EXPRESSION TAG	UNP Q12657
C	215	HIS	-	EXPRESSION TAG	UNP Q12657
C	216	HIS	-	EXPRESSION TAG	UNP Q12657

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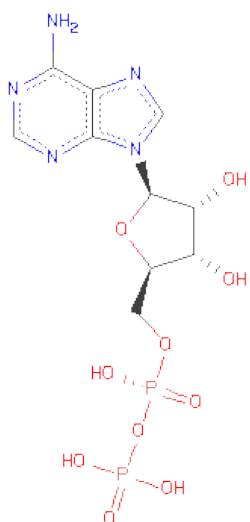
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Chain	Residue	Modelled	Actual	Comment	Reference
C	217	HIS	-	EXPRESSION TAG	UNP Q12657
C	218	HIS	-	EXPRESSION TAG	UNP Q12657
C	219	HIS	-	EXPRESSION TAG	UNP Q12657
D	212	LEU	-	EXPRESSION TAG	UNP Q12657
D	213	GLU	-	EXPRESSION TAG	UNP Q12657
D	214	HIS	-	EXPRESSION TAG	UNP Q12657
D	215	HIS	-	EXPRESSION TAG	UNP Q12657
D	216	HIS	-	EXPRESSION TAG	UNP Q12657
D	217	HIS	-	EXPRESSION TAG	UNP Q12657
D	218	HIS	-	EXPRESSION TAG	UNP Q12657
D	219	HIS	-	EXPRESSION TAG	UNP Q12657

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

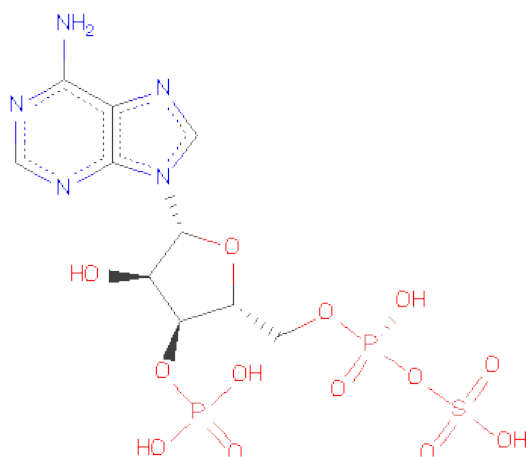
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 3'-PHOSPHATE-ADENOSINE-5'-PHOSPHATESULFATE (three-letter code: PPS) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>13</sub>P<sub>2</sub>S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	121	Total	O	0	0
			121	121		
5	C	105	Total	O	0	0
			105	105		

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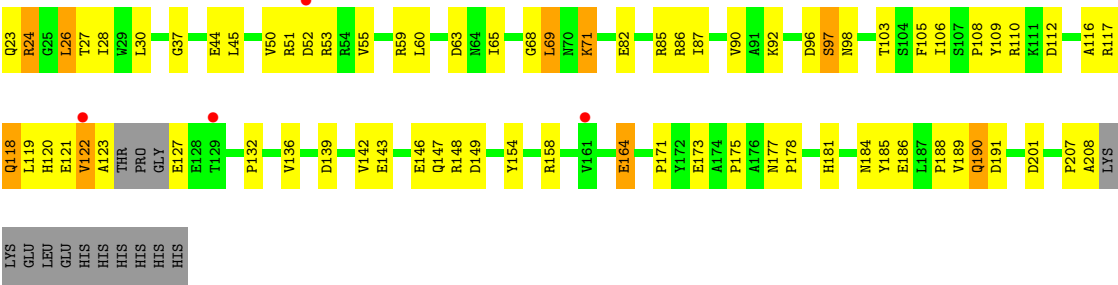
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	138	Total 138	O 138	0	0



● Molecule 1: Adenylyl-sulfate kinase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.58Å 82.59Å 139.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.71 – 2.50 31.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (31.71-2.50) 99.4 (31.72-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.198 , 0.279 0.239 , 0.265	Depositor DCC
$R_{free}$ test set	1280 reflections (4.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 31401 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1286e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.47	0/1415	0.69	0/1921
1	B	0.51	1/1432 (0.1%)	0.65	0/1942
1	C	0.52	1/1398 (0.1%)	0.69	2/1898 (0.1%)
1	D	0.49	0/1425	0.66	0/1940
All	All	0.50	2/5670 (0.0%)	0.68	2/7701 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	58	TYR	C-O	-11.44	1.01	1.23
1	B	147	GLN	CB-CG	-5.26	1.38	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	TYR	O-C-N	-6.04	113.04	122.70
1	C	58	TYR	CA-C-O	5.58	131.82	120.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1388	0	1357	91	0
1	B	1407	0	1383	61	1
1	C	1370	0	1317	89	0
1	D	1397	0	1344	73	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	4	0
3	C	27	0	12	3	0
3	D	27	0	12	11	0
4	A	31	0	12	4	0
4	C	31	0	12	1	0
5	A	131	0	0	14	0
5	B	121	0	0	7	0
5	C	105	0	0	11	0
5	D	138	0	0	11	0
All	All	6230	0	5473	317	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 317 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:23:GLN:O	1:D:98:ASN:ND2	1.73	1.19
1:C:110[B]:ARG:NH1	1:C:176:ALA:H	1.48	1.11
1:D:51:ARG:HG2	1:D:52:ASP:OD1	1.47	1.11
1:A:51:ARG:HG2	1:A:52:ASP:OD1	1.57	1.02
1:C:110[B]:ARG:HH12	1:C:176:ALA:N	1.56	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:147:GLN:NE2	1:D:147:GLN:NE2[2_564]	1.70	0.50

## 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	175/197 (89%)	158 (90%)	16 (9%)	1 (1%)	33	55
1	B	177/197 (90%)	167 (94%)	10 (6%)	0	100	100
1	C	175/197 (89%)	157 (90%)	16 (9%)	2 (1%)	21	34
1	D	180/197 (91%)	165 (92%)	15 (8%)	0	100	100
All	All	707/788 (90%)	647 (92%)	57 (8%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	THR
1	A	189	VAL
1	C	54	ARG

### 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	143/168 (85%)	129 (90%)	14 (10%)	12	21
1	B	146/168 (87%)	132 (90%)	14 (10%)	12	22
1	C	139/168 (83%)	126 (91%)	13 (9%)	13	23
1	D	142/168 (84%)	128 (90%)	14 (10%)	11	21
All	All	570/672 (85%)	515 (90%)	55 (10%)	12	22

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	177	ASN
1	C	47	HIS
1	D	164	GLU
1	B	190	GLN
1	B	202	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	181	HIS
1	B	184	ASN
1	C	184	ASN
1	B	120	HIS
1	B	177	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	2001	-	29,29,29	1.09	1 (3%)	45,45,45	1.82	7 (15%)
4	PPS	A	2002	-	33,33,33	5.14	21 (63%)	51,52,52	2.02	9 (17%)
3	ADP	B	2003	-	29,29,29	1.18	2 (6%)	45,45,45	1.98	8 (17%)
3	ADP	C	2004	-	29,29,29	1.23	2 (6%)	45,45,45	1.93	9 (20%)
4	PPS	C	2005	-	33,33,33	5.23	22 (66%)	51,52,52	2.42	11 (21%)
3	ADP	D	2006	-	29,29,29	1.22	2 (6%)	45,45,45	2.17	13 (28%)

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	2001	-	-	0/16/32/32	0/1/3/3
4	PPS	A	2002	-	-	0/17/37/37	0/1/3/3
3	ADP	B	2003	-	-	0/16/32/32	0/1/3/3
3	ADP	C	2004	-	-	0/16/32/32	0/1/3/3
4	PPS	C	2005	-	-	1/17/37/37	0/1/3/3
3	ADP	D	2006	-	-	0/16/32/32	0/1/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2002	PPS	C2-N3	12.75	1.57	1.32
4	C	2005	PPS	C2-N3	12.33	1.56	1.32
4	C	2005	PPS	C8-N9	11.80	1.54	1.36
4	A	2002	PPS	C8-N9	11.18	1.53	1.36
4	A	2002	PPS	C4-N3	10.92	1.52	1.35

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2005	PPS	N3-C2-N1	-11.31	119.25	128.71
4	A	2002	PPS	N3-C2-N1	-10.16	120.22	128.71
4	C	2005	PPS	O4'-C1'-N9	-8.70	100.35	108.44
3	B	2003	ADP	N3-C2-N1	-7.47	122.46	128.71
3	C	2004	ADP	N3-C2-N1	-6.89	122.94	128.71

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2005	PPS	P1-O3'-C3'-C4'

There are no ring outliers.

## 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 ⓘ

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	179/197 (90%)	0.14	2 (1%) 77 79	16, 35, 68, 130	6 (3%)
1	B	181/197 (91%)	-0.02	3 (1%) 67 69	13, 33, 58, 90	4 (2%)
1	C	178/197 (90%)	0.10	7 (3%) 37 38	19, 36, 72, 114	1 (0%)
1	D	183/197 (92%)	-0.12	4 (2%) 59 61	15, 31, 69, 100	1 (0%)
All	All	721/788 (91%)	0.02	16 (2%) 59 61	13, 34, 70, 130	12 (1%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	THR	4.6
1	A	107	SER	3.4
1	D	52	ASP	3.0
1	D	129	THR	2.8
1	D	161	VAL	2.5

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	D	2006	27/27	0.14	0.89	5,22,72,118	0
4	PPS	C	2005	31/31	0.16	0.30	0,28,94,247	0
2	CL	B	502	1/1	0.15	0.25	31,31,31,31	0
3	ADP	C	2004	27/27	0.12	-0.61	13,39,89,263	0
4	PPS	A	2002	31/31	0.14	-0.61	7,29,91,116	0
3	ADP	A	2001	27/27	0.13	-0.69	0,37,86,162	0
3	ADP	B	2003	27/27	0.11	-0.82	4,25,50,57	0
2	CL	A	503	1/1	0.04	-2.10	22,22,22,22	0
2	CL	C	501	1/1	0.09	-2.60	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.