



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:52 PM GMT

PDB ID : 1QVR  
Title : Crystal Structure Analysis of ClpB  
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Deposited on : 2003-08-28  
Resolution : 3.00 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  
<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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

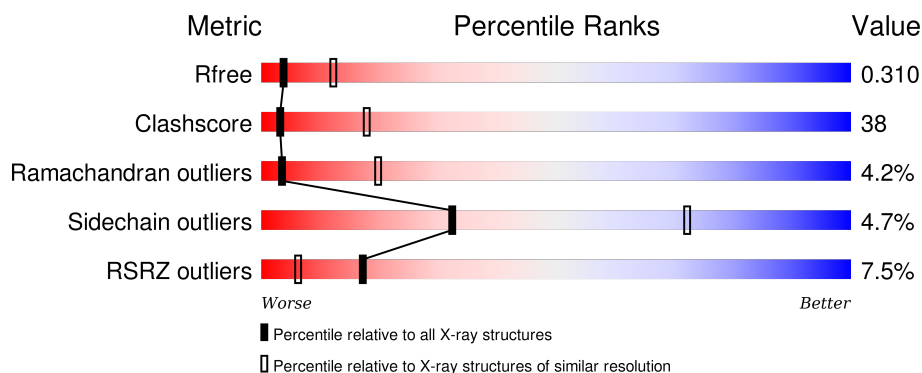
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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.

Mol	Chain	Length	Quality of chain
1	A	854	<div> <div>5%</div> <div>39%</div> <div>50%</div> <div>5%</div> <div>6%</div> </div>
1	B	854	<div> <div>2%</div> <div>39%</div> <div>50%</div> <div>5%</div> <div>6%</div> </div>
1	C	854	<div> <div>14%</div> <div>41%</div> <div>48%</div> <div>•</div> <div>6%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19496 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.

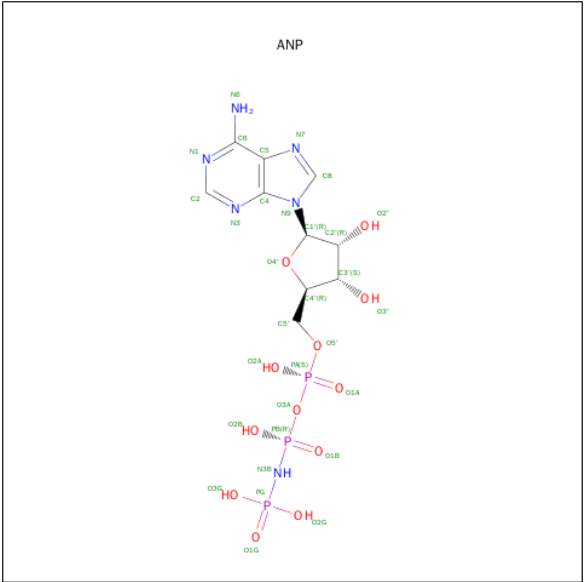
- Molecule 1 is a protein called ClpB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	803	Total	C	N	O	S	0	0	0
			6429	4050	1168	1204	7			
1	B	803	Total	C	N	O	S	0	0	0
			6429	4050	1168	1204	7			
1	C	803	Total	C	N	O	S	0	0	0
			6429	4050	1168	1204	7			

- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

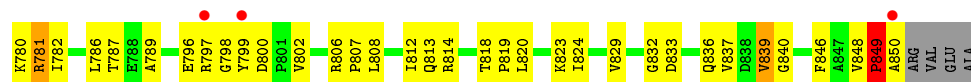
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	8	Total	Pt	0	0
			8	8		
2	A	8	Total	Pt	0	0
			8	8		
2	C	7	Total	Pt	0	0
			7	7		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

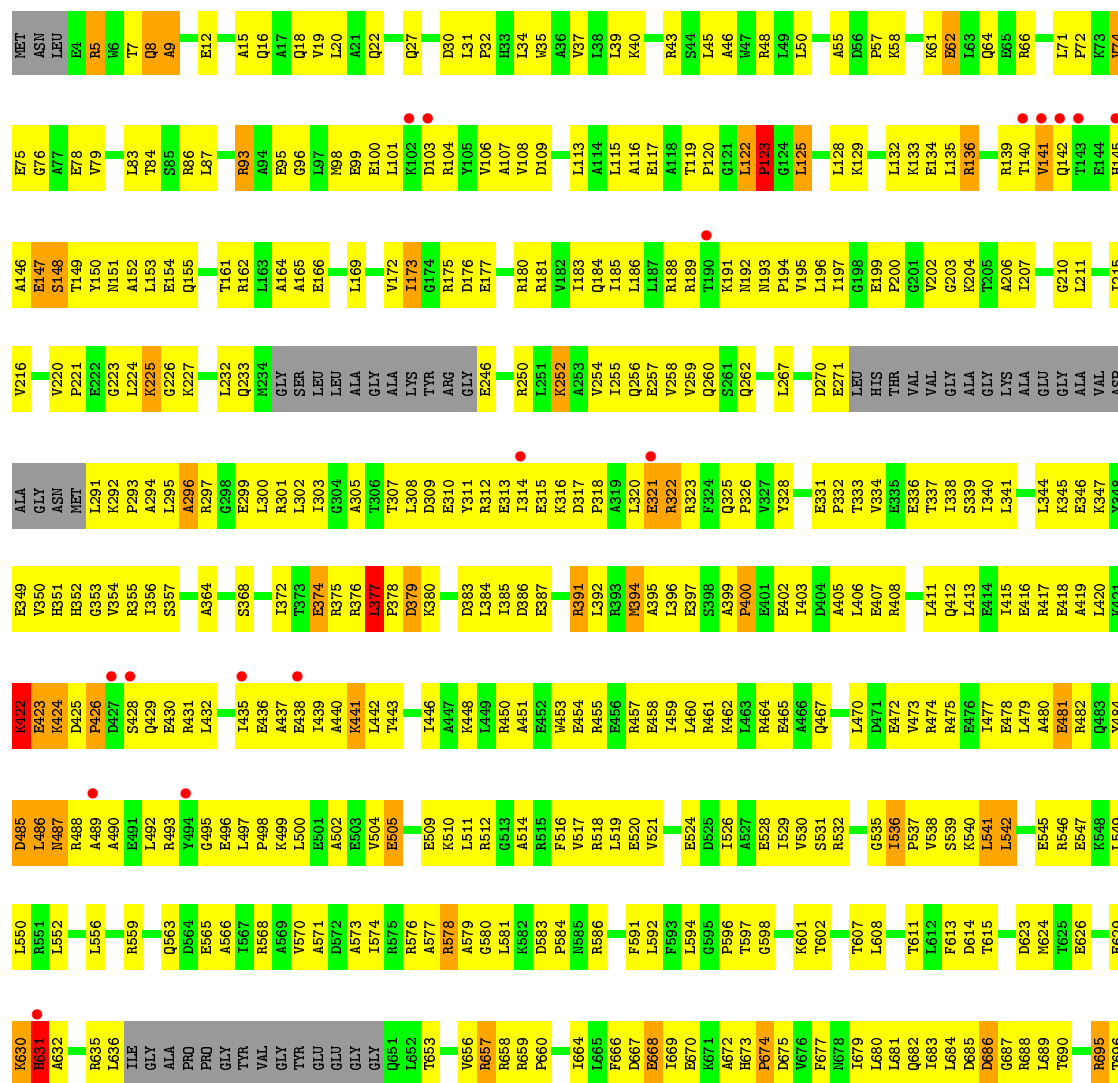


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

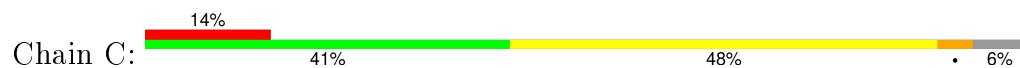


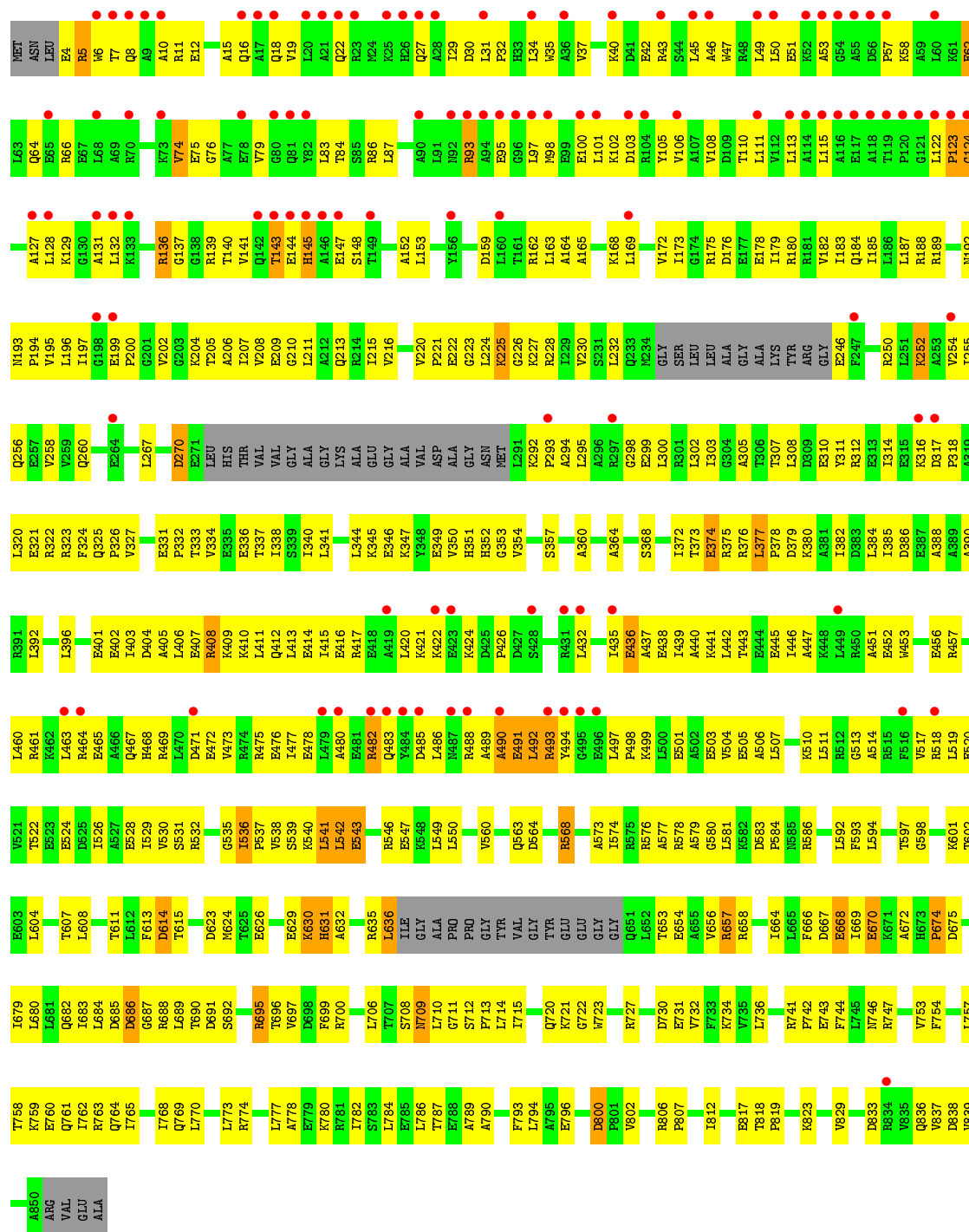


• Molecule 1: ClpB protein



• Molecule 1: ClpB protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.75Å 138.48Å 212.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 3.00 48.04 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.4 (48.04-3.00) 88.5 (48.04-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.263 , 0.307 0.265 , 0.310	Depositor DCC
$R_{free}$ test set	2643 reflections (4.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 74.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 108756 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ANP, PT

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	0/6513	0.57	2/8778 (0.0%)
1	B	0.31	0/6513	0.60	7/8778 (0.1%)
1	C	0.28	0/6513	0.57	1/8778 (0.0%)
All	All	0.29	0/19539	0.58	10/26334 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	659	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	658	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	658	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	781	ARG	NE-CZ-NH2	5.41	123.01	120.30

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	6429	0	6642	517	0
1	B	6429	0	6643	530	0
1	C	6429	0	6642	475	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	7	0	0	0	0
3	A	62	0	26	9	0
3	B	62	0	26	5	0
3	C	62	0	26	5	0
All	All	19496	0	20005	1495	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 38.

The worst 5 of 1495 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:C:165:ALA:HA	1:C:216:VAL:HG11	1.32	1.10
1:A:20:LEU:HB2	1:A:262:GLN:HE22	1.20	1.05
1:A:839:VAL:HG22	1:A:840:GLY:H	1.20	1.04
1:A:5:ARG:HD2	1:A:6:TRP:H	1.25	0.99
1:B:175:ARG:HD3	1:B:207:ILE:HD11	1.44	0.97

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	795/854 (93%)	666 (84%)	93 (12%)	36 (4%)	3	18
1	B	795/854 (93%)	655 (82%)	104 (13%)	36 (4%)	3	18
1	C	795/854 (93%)	659 (83%)	108 (14%)	28 (4%)	4	24
All	All	2385/2562 (93%)	1980 (83%)	305 (13%)	100 (4%)	3	20

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLY
1	A	123	PRO
1	A	141	VAL
1	A	374	GLU
1	A	377	LEU

### 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	675/706 (96%)	644 (95%)	31 (5%)	33	73
1	B	675/706 (96%)	641 (95%)	34 (5%)	30	70
1	C	675/706 (96%)	645 (96%)	30 (4%)	35	74
All	All	2025/2118 (96%)	1930 (95%)	95 (5%)	32	72

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

Mol	Chain	Res	Type
1	B	225	LYS
1	B	614	ASP
1	C	674	PRO
1	B	252	LYS
1	B	429	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	HIS
1	B	325	GLN
1	C	682	GLN
1	B	256	GLN
1	B	351	HIS

### 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 29 ligands modelled in this entry, 23 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	ANP	A	901	-	27,33,33	2.16	8 (29%)	30,52,52	2.84	8 (26%)
3	ANP	A	911	-	27,33,33	1.92	7 (25%)	30,52,52	2.76	8 (26%)
3	ANP	B	902	-	27,33,33	1.98	7 (25%)	30,52,52	2.81	8 (26%)
3	ANP	B	912	-	27,33,33	1.86	8 (29%)	30,52,52	2.82	9 (30%)
3	ANP	C	903	-	27,33,33	1.97	7 (25%)	30,52,52	2.83	8 (26%)
3	ANP	C	913	-	27,33,33	1.83	7 (25%)	30,52,52	2.79	8 (26%)

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	ANP	A	901	-	-	0/12/38/38	0/3/3/3
3	ANP	A	911	-	-	0/12/38/38	0/3/3/3
3	ANP	B	902	-	-	0/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	B	912	-	-	1/12/38/38	0/3/3/3
3	ANP	C	903	-	-	0/12/38/38	0/3/3/3
3	ANP	C	913	-	-	0/12/38/38	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	ANP	PB-O2B	-3.98	1.45	1.56
3	B	902	ANP	PB-O2B	-3.91	1.45	1.56
3	A	901	ANP	PB-O2B	-3.66	1.46	1.56
3	B	912	ANP	PB-O2B	-3.52	1.46	1.56
3	A	911	ANP	PB-O2B	-3.24	1.47	1.56

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	ANP	O1B-PB-N3B	-6.72	101.59	111.90
3	C	903	ANP	N3-C2-N1	-6.65	123.80	128.89
3	A	911	ANP	N3-C2-N1	-6.63	123.82	128.89
3	A	901	ANP	O1B-PB-N3B	-6.52	101.89	111.90
3	C	913	ANP	N3-C2-N1	-6.50	123.92	128.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	912	ANP	O1G-PG-N3B-PB

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ANP	3	0
3	A	911	ANP	6	0
3	B	902	ANP	3	0
3	B	912	ANP	2	0
3	C	903	ANP	2	0
3	C	913	ANP	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](#)

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	803/854 (94%)	0.24	45 (5%) 28 11	32, 93, 142, 187	0
1	B	803/854 (94%)	0.14	18 (2%) 65 35	33, 82, 134, 176	0
1	C	803/854 (94%)	0.73	117 (14%) 3 1	37, 108, 171, 192	0
All	All	2409/2562 (94%)	0.37	180 (7%) 17 6	32, 92, 162, 192	0

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124	GLY	10.6
1	C	46	ALA	10.0
1	C	25	LYS	8.6
1	C	50	LEU	7.9
1	C	123	PRO	7.4

### 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ANP	C	913	31/31	0.92	0.27	0.41	31,66,117,121	0
3	ANP	B	902	31/31	0.93	0.27	0.22	64,80,143,146	0
3	ANP	C	903	31/31	0.85	0.30	0.08	114,149,172,173	0
2	PT	C	857	1/1	0.96	0.27	-0.05	41,41,41,41	1
3	ANP	A	911	31/31	0.92	0.24	-0.07	55,79,110,119	0
3	ANP	B	912	31/31	0.93	0.23	-0.23	42,71,130,136	0
3	ANP	A	901	31/31	0.91	0.20	-0.63	75,108,124,130	0
2	PT	A	861	1/1	0.80	0.18	-1.14	45,45,45,45	1
2	PT	A	862	1/1	0.97	0.13	-1.39	53,53,53,53	1
2	PT	B	861	1/1	0.95	0.14	-1.41	47,47,47,47	1
2	PT	C	856	1/1	0.89	0.15	-1.44	19,19,19,19	1
2	PT	B	857	1/1	0.96	0.50	-	16,16,16,16	1
2	PT	B	858	1/1	0.92	0.60	-	31,31,31,31	1
2	PT	C	855	1/1	0.93	0.37	-	46,46,46,46	1
2	PT	A	860	1/1	0.86	0.45	-	66,66,66,66	1
2	PT	C	860	1/1	0.91	0.20	-	90,90,90,90	1
2	PT	A	859	1/1	0.91	0.32	-	59,59,59,59	1
2	PT	C	858	1/1	0.89	0.12	-	80,80,80,80	1
2	PT	B	859	1/1	0.92	0.24	-	50,50,50,50	1
2	PT	B	855	1/1	0.98	0.47	-	54,54,54,54	1
2	PT	A	855	1/1	0.95	0.42	-	52,52,52,52	1
2	PT	A	858	1/1	0.95	0.29	-	49,49,49,49	1
2	PT	A	856	1/1	0.96	0.33	-	69,69,69,69	1
2	PT	C	859	1/1	0.86	0.25	-	51,51,51,51	1
2	PT	B	856	1/1	0.98	0.35	-	39,39,39,39	1
2	PT	C	861	1/1	0.91	0.30	-	42,42,42,42	1
2	PT	A	857	1/1	0.89	0.58	-	44,44,44,44	1
2	PT	B	862	1/1	0.87	0.48	-	52,52,52,52	1
2	PT	B	860	1/1	0.86	0.74	-	34,34,34,34	1

## 6.5 Other polymers

There are no such residues in this entry.