



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2016 – 07:32 AM EDT

PDB ID : 5JCH  
Title : Crystal structure of chicken MDA5 with 5'p 10-mer dsRNA and ADP-Mg2+  
at 2.95 Å resolution (untwinned).  
Authors : Cusack, S.; Uchikawa, E.  
Deposited on : 2016-04-15  
Resolution : 2.95 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027457  
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) : rb-20027457

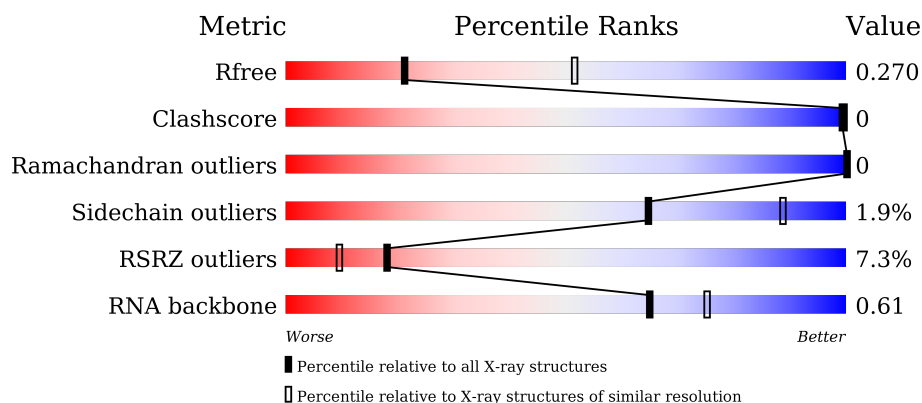
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)
RNA backbone	2183	1010 (3.36-2.56)

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	701	<div> <div>5%</div> <div>91%</div> <div>6%</div> </div>
1	B	701	<div> <div>9%</div> <div>90%</div> <div>7%</div> </div>
2	U	10	<div> <div>90%</div> <div>10%</div> </div>
2	V	10	<div> <div>90%</div> <div>10%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	X	10	 80%20%
2	Y	10	 90%10%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11661 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 Melanoma differentiation associated protein-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5396	3403	967	994	32			
1	B	655	Total	C	N	O	S	0	0	0
			5353	3376	959	986	32			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLY	-	expression tag	UNP D9N195
A	295	ALA	-	expression tag	UNP D9N195
A	296	MET	-	expression tag	UNP D9N195
A	297	GLY	-	expression tag	UNP D9N195
A	436	GLN	GLU	engineered mutation	UNP D9N195
B	294	GLY	-	expression tag	UNP D9N195
B	295	ALA	-	expression tag	UNP D9N195
B	296	MET	-	expression tag	UNP D9N195
B	297	GLY	-	expression tag	UNP D9N195
B	436	GLN	GLU	engineered mutation	UNP D9N195

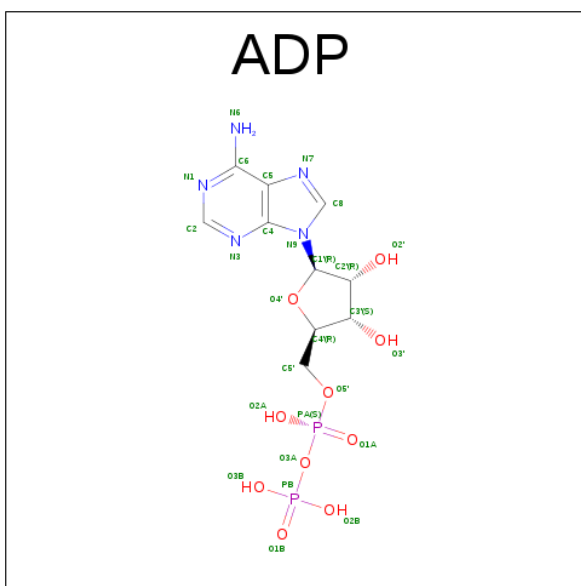
- Molecule 2 is a RNA chain called RNA (5'-R(P\*GP\*GP\*UP\*AP\*CP\*GP\*UP\*AP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	10	Total	C	N	O	P	0	0	0
			214	95	38	71	10			
2	Y	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			
2	U	10	Total	C	N	O	P	0	0	0
			214	95	38	71	10			
2	V	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			


- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 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>).






Chain Y:  90% 10%




- Molecule 2: RNA (5'-R(P\*GP\*GP\*UP\*AP\*CP\*GP\*UP\*AP\*CP\*C)-3')

Chain U:  90% 10%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*UP\*AP\*CP\*GP\*UP\*AP\*CP\*C)-3')

Chain V:  90% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.08 Å 139.73 Å 103.19 Å 90.00° 110.14° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 48.61 – 2.95	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.95) 94.2 (48.61-2.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.96 Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.256 , 0.270 0.260 , 0.270	Depositor DCC
$R_{free}$ test set	1907 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	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 24.60 % 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 3.7162e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.36	0/5482	0.56	1/7353 (0.0%)
1	B	0.37	0/5438	0.56	1/7293 (0.0%)
2	U	0.69	1/238 (0.4%)	0.69	0/367
2	V	0.20	0/237	0.70	0/367
2	X	0.68	1/238 (0.4%)	0.67	0/367
2	Y	0.20	0/237	0.70	0/367
All	All	0.38	2/11870 (0.0%)	0.57	2/16114 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	1	G	OP3-P	-10.25	1.48	1.61
2	X	1	G	OP3-P	-10.06	1.49	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	536	ASP	CB-CG-OD2	5.14	122.93	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	5396	0	5482	6	0
1	B	5353	0	5438	5	0
2	U	214	0	109	0	0
2	V	213	0	109	0	0
2	X	214	0	109	0	0
2	Y	213	0	109	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	11661	0	11380	11	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 0.

All (11) 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:308:VAL:HG11	1:B:320:ILE:HG23	1.87	0.57
1:A:308:VAL:HG11	1:A:320:ILE:HG23	1.87	0.56
1:B:383:LEU:HD11	1:B:396:VAL:HG11	1.93	0.51
1:A:383:LEU:HD11	1:A:396:VAL:HG11	1.93	0.51
1:A:778:VAL:CG1	1:A:797:ALA:HB2	2.45	0.47
1:B:778:VAL:CG1	1:B:797:ALA:HB2	2.45	0.47
1:A:609:ILE:HD11	1:A:704:SER:CB	2.46	0.45
1:B:609:ILE:HD11	1:B:704:SER:CB	2.46	0.45
1:A:436:GLN:OE1	1:A:436:GLN:HA	2.19	0.43
1:B:686:GLU:HG2	1:B:777:ILE:HB	2.02	0.41
1:A:686:GLU:HG2	1:A:777:ILE:HB	2.02	0.41

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	647/701 (92%)	619 (96%)	28 (4%)	0	100	100
1	B	641/701 (91%)	615 (96%)	26 (4%)	0	100	100
All	All	1288/1402 (92%)	1234 (96%)	54 (4%)	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	595/630 (94%)	585 (98%)	10 (2%)	68	90
1	B	590/630 (94%)	578 (98%)	12 (2%)	63	88
All	All	1185/1260 (94%)	1163 (98%)	22 (2%)	65	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	LYS
1	A	529	LYS
1	A	598	LYS
1	A	609	ILE
1	A	694	ARG
1	A	715	ASN
1	A	778	VAL
1	A	852	LEU
1	A	885	HIS
1	A	945	ASN
1	B	328	LYS
1	B	529	LYS
1	B	535	ASP
1	B	598	LYS
1	B	609	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	653	ARG
1	B	694	ARG
1	B	715	ASN
1	B	778	VAL
1	B	852	LEU
1	B	885	HIS
1	B	945	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
1	A	447	ASN
1	A	554	GLN
1	B	441	GLN
1	B	554	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	U	9/10 (90%)	0	0
2	V	9/10 (90%)	1 (11%)	0
2	X	9/10 (90%)	1 (11%)	0
2	Y	9/10 (90%)	1 (11%)	0
All	All	36/40 (90%)	3 (8%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	10	C
2	Y	4	A
2	V	4	A

There are no RNA pucker outliers to report.

## 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
4	ADP	A	1002	5	24,29,29	1.05	1 (4%)	23,45,45	1.93	2 (8%)
4	ADP	B	1002	5	24,29,29	1.07	2 (8%)	23,45,45	1.90	1 (4%)

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
4	ADP	A	1002	5	-	0/12/32/32	0/3/3/3
4	ADP	B	1002	5	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	ADP	C2-N3	2.03	1.35	1.32
4	B	1002	ADP	C5-C4	3.25	1.47	1.40
4	A	1002	ADP	C5-C4	3.29	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	N3-C2-N1	-7.82	122.73	128.87
4	B	1002	ADP	N3-C2-N1	-7.73	122.80	128.87
4	A	1002	ADP	C4'-O4'-C1'	2.10	111.86	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	661/701 (94%)	0.44	37 (5%) 28 15	38, 74, 114, 134	0
1	B	655/701 (93%)	0.57	62 (9%) 10 5	39, 82, 132, 155	0
2	U	10/10 (100%)	0.17	0 100 100	48, 58, 70, 80	0
2	V	10/10 (100%)	-0.01	0 100 100	53, 58, 66, 87	0
2	X	10/10 (100%)	0.24	0 100 100	44, 54, 67, 69	0
2	Y	10/10 (100%)	0.32	0 100 100	50, 54, 59, 73	0
All	All	1356/1442 (94%)	0.49	99 (7%) 18 9	38, 78, 125, 155	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	951	GLY	8.2
1	A	885	HIS	6.0
1	B	690	THR	5.9
1	B	463	GLN	5.2
1	B	957	LEU	4.9
1	A	892	GLU	4.7
1	B	905	VAL	4.6
1	B	935	ILE	4.6
1	B	967	GLU	4.6
1	B	885	HIS	4.6
1	B	879	PHE	4.5
1	B	465	LYS	4.4
1	A	465	LYS	4.2
1	B	470	LEU	4.0
1	B	894	ILE	3.9
1	A	536	ASP	3.9
1	B	685	GLU	3.9
1	A	463	GLN	3.8
1	A	894	ILE	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	904	SER	3.8
1	A	462	LYS	3.8
1	B	949	TYR	3.8
1	B	466	GLU	3.8
1	B	897	ILE	3.7
1	B	948	VAL	3.7
1	B	422	GLU	3.7
1	A	912	LEU	3.7
1	A	967	GLU	3.6
1	B	349	GLN	3.6
1	A	470	LEU	3.6
1	B	536	ASP	3.5
1	B	947	MET	3.5
1	B	977	LYS	3.5
1	B	634	ASP	3.4
1	A	876	LEU	3.2
1	B	631	ALA	3.1
1	B	633	SER	3.0
1	B	984	ILE	3.0
1	A	950	ARG	3.0
1	B	911	HIS	3.0
1	B	716	PRO	2.9
1	A	951	GLY	2.9
1	B	929	GLN	2.9
1	A	608	THR	2.8
1	A	935	ILE	2.8
1	A	955	PRO	2.8
1	B	655	PHE	2.8
1	B	986	PHE	2.8
1	A	634	ASP	2.7
1	A	466	GLU	2.7
1	B	464	ALA	2.7
1	B	627	ARG	2.7
1	B	953	ASP	2.7
1	B	954	LEU	2.7
1	B	909	PHE	2.6
1	B	618	LEU	2.6
1	A	691	GLU	2.6
1	B	691	GLU	2.6
1	A	905	VAL	2.6
1	B	632	GLU	2.6
1	B	950	ARG	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	957	LEU	2.5
1	A	903	VAL	2.5
1	B	565	PHE	2.5
1	A	677	MET	2.5
1	A	913	TYR	2.4
1	B	564	GLU	2.4
1	A	904	SER	2.4
1	A	633	SER	2.4
1	A	954	LEU	2.4
1	B	867	ARG	2.4
1	B	903	VAL	2.4
1	B	972	THR	2.4
1	A	874	PRO	2.4
1	B	930	THR	2.3
1	B	916	ARG	2.3
1	B	530	LYS	2.3
1	B	626	LYS	2.3
1	A	530	LYS	2.3
1	A	953	ASP	2.3
1	B	462	LYS	2.3
1	B	402	VAL	2.2
1	B	913	TYR	2.2
1	B	625	LEU	2.2
1	B	677	MET	2.2
1	B	960	ARG	2.2
1	B	955	PRO	2.2
1	B	617	HIS	2.2
1	A	388	GLU	2.2
1	B	861	LYS	2.1
1	A	968	ASP	2.1
1	B	978	LYS	2.1
1	A	671	TYR	2.1
1	A	900	MET	2.1
1	B	692	GLU	2.0
1	B	656	HIS	2.0
1	A	934	ILE	2.0
1	A	872	LYS	2.0
1	A	887	LEU	2.0

## 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 [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
4	ADP	B	1002	27/27	0.90	0.19	-0.33	101,104,110,111	0
4	ADP	A	1002	27/27	0.92	0.15	-0.92	81,87,100,101	0
3	ZN	A	1001	1/1	0.98	0.14	-1.87	74,74,74,74	0
3	ZN	B	1001	1/1	0.98	0.09	-2.34	100,100,100,100	0
5	MG	B	1003	1/1	0.97	0.08	-	46,46,46,46	0
5	MG	A	1003	1/1	0.95	0.11	-	53,53,53,53	0

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

There are no such residues in this entry.