



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2017 – 05:04 PM EDT

PDB ID : 5XDR  
Title : Crystal structure of human DEAH-box RNA helicase DHX15 in complex with ADP  
Authors : Murakami, K.; Nakano, K.; Shimizu, T.; Ohto, U.  
Deposited on : 2017-03-29  
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029077

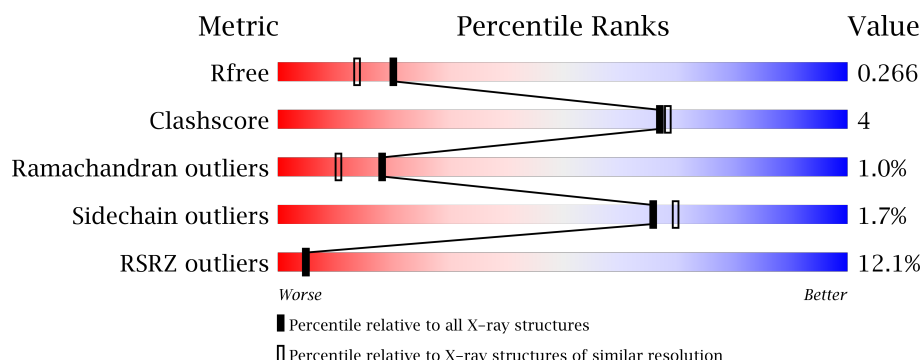
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	690	<div> <div>12%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5586 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.

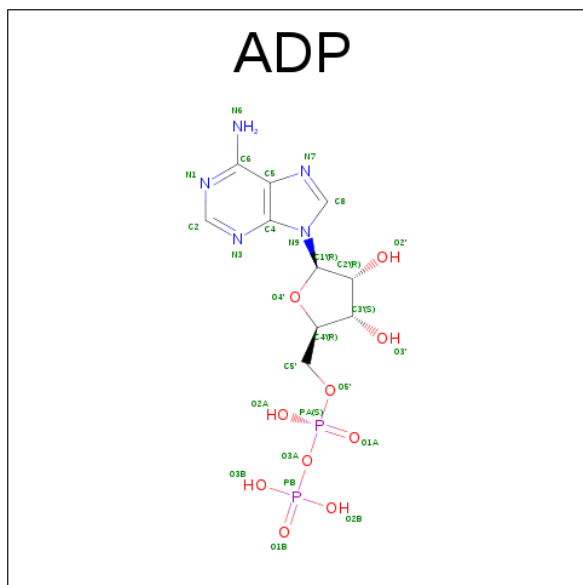
- Molecule 1 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	679	5458	3467	941	1014	36	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

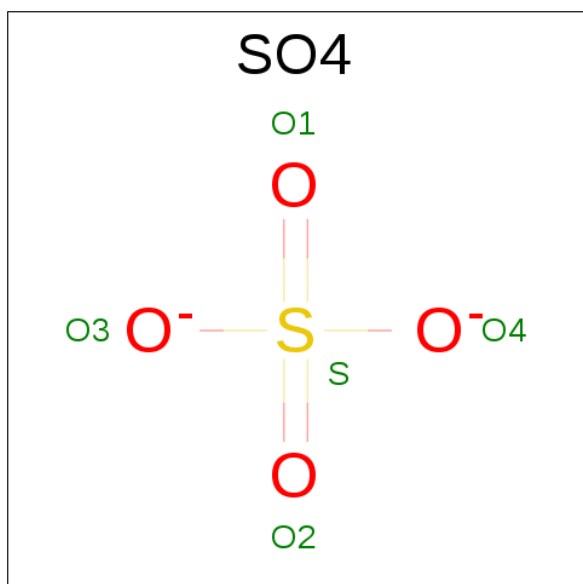
Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	expression tag	UNP O43143
A	107	PRO	-	expression tag	UNP O43143
A	108	GLU	-	expression tag	UNP O43143
A	109	PHE	-	expression tag	UNP O43143
A	678	SER	THR	engineered mutation	UNP O43143

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

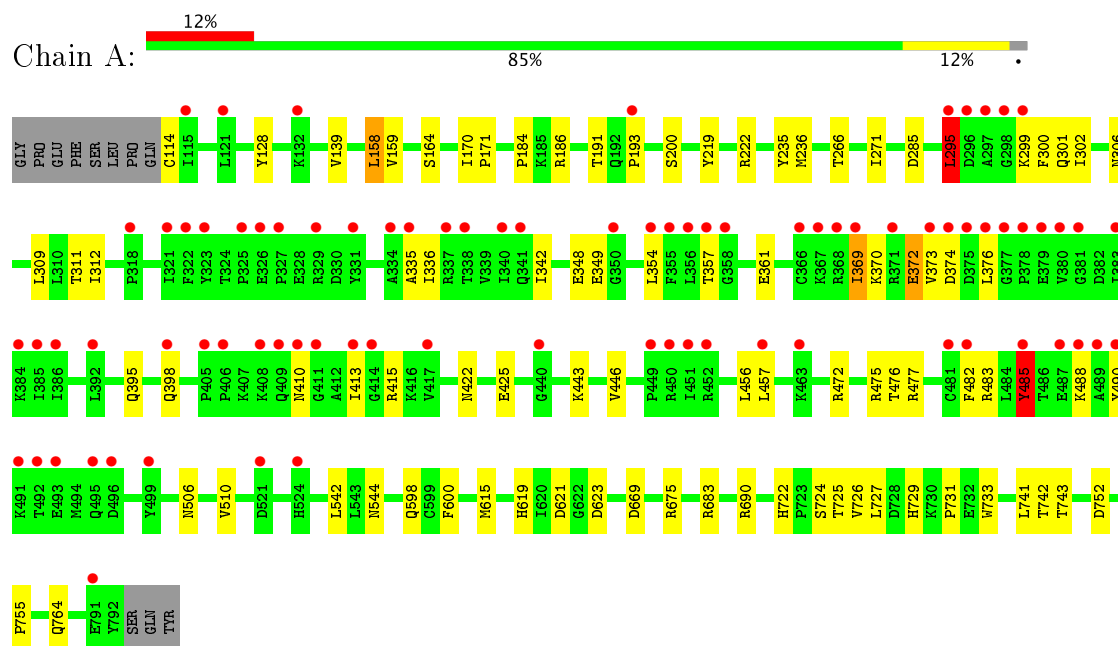
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		

### 3 Residue-property plots [i](#)

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.

- Molecule 1: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX15



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.92Å 89.38Å 211.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.54 – 2.00 45.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (105.54-2.00) 100.0 (45.83-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.223 , 0.269 0.228 , 0.266	Depositor DCC
$R_{free}$ test set	2649 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, SO4, 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	0.68	0/5573	0.85	10/7553 (0.1%)

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	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	690	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	690	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	222	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	675	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	222	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	669	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	752	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	158	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	295	LEU	CB-CG-CD1	5.25	119.92	111.00
1	A	485	TYR	CA-CB-CG	5.22	123.33	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	ASP	Peptide

## 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	5458	0	5480	49	0
2	A	27	0	12	1	0
3	A	10	0	0	0	0
4	A	1	0	0	0	0
5	A	90	0	0	0	1
All	All	5586	0	5492	49	1

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 4.

All (49) 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:598:GLN:HE21	1:A:600:PHE:H	1.20	0.90
1:A:725:THR:HG22	1:A:727:LEU:H	1.48	0.79
1:A:623:ASP:OD2	1:A:725:THR:HG23	1.90	0.71
1:A:139:VAL:HG12	1:A:312:ILE:HD13	1.77	0.67
1:A:544:ASN:ND2	1:A:764:GLN:HE22	1.96	0.62
1:A:544:ASN:HD21	1:A:764:GLN:HE22	1.50	0.60
1:A:619:HIS:HD2	1:A:621:ASP:H	1.48	0.60
1:A:369:ILE:HD12	1:A:369:ILE:N	2.20	0.56
1:A:271:ILE:CD1	1:A:510:VAL:HG22	2.36	0.55
1:A:186:ARG:NH1	1:A:285:ASP:OD2	2.36	0.55
1:A:619:HIS:CD2	1:A:621:ASP:H	2.26	0.54
1:A:299:LYS:HG2	1:A:302:ILE:HD13	1.89	0.52
1:A:200:SER:HB2	1:A:398:GLN:HE22	1.75	0.52
1:A:370:LYS:N	1:A:372:GLU:O	2.44	0.51
1:A:425:GLU:O	1:A:472:ARG:NH1	2.43	0.51
1:A:159:VAL:HG23	1:A:311:THR:HG23	1.93	0.50
1:A:193:PRO:HB3	1:A:266:THR:HG21	1.93	0.49
1:A:114:CYS:N	1:A:128:TYR:HH	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:TRP:CE2	1:A:755:PRO:HB3	2.47	0.49
1:A:369:ILE:HG22	1:A:369:ILE:O	2.13	0.49
1:A:200:SER:CB	1:A:398:GLN:HE22	2.25	0.48
1:A:336:ILE:HG21	1:A:369:ILE:HD11	1.96	0.47
1:A:139:VAL:HG13	1:A:164:SER:O	2.15	0.47
1:A:159:VAL:HG22	1:A:309:LEU:HD11	1.95	0.47
1:A:299:LYS:O	1:A:301:GLN:N	2.48	0.46
1:A:372:GLU:HG2	1:A:373:VAL:HA	1.97	0.46
1:A:219:TYR:HA	1:A:235:TYR:O	2.16	0.46
1:A:446:VAL:HG22	1:A:457:LEU:HD23	1.98	0.46
1:A:349:GLU:HA	1:A:413:ILE:HG21	1.99	0.45
1:A:335:ALA:HB1	1:A:354:LEU:HD11	1.99	0.44
1:A:542:LEU:C	1:A:542:LEU:HD23	2.37	0.44
1:A:302:ILE:HG13	1:A:306:ASN:HD21	1.81	0.44
1:A:722:HIS:HD2	1:A:724:SER:OG	2.00	0.44
1:A:598:GLN:HE21	1:A:600:PHE:N	2.01	0.44
1:A:369:ILE:C	1:A:372:GLU:O	2.56	0.43
1:A:615:MET:CE	1:A:726:VAL:HG12	2.48	0.43
1:A:742:THR:HG22	1:A:743:THR:H	1.83	0.43
1:A:348:GLU:O	1:A:415:ARG:NH2	2.51	0.43
1:A:729:HIS:O	1:A:731:PRO:HD3	2.19	0.43
1:A:170:ILE:HB	1:A:171:PRO:HD3	2.01	0.42
1:A:295:LEU:N	1:A:295:LEU:CD1	2.82	0.42
1:A:342:ILE:HD11	1:A:482:PHE:CD2	2.54	0.42
1:A:475:ARG:NH2	2:A:801:ADP:O3'	2.53	0.41
1:A:476:THR:HG21	1:A:477:ARG:HH21	1.85	0.41
1:A:483:ARG:HB3	1:A:485:TYR:CD2	2.55	0.41
1:A:357:THR:HG22	1:A:361:GLU:OE1	2.20	0.41
1:A:598:GLN:HE22	1:A:600:PHE:HD2	1.69	0.41
1:A:357:THR:OG1	1:A:443:LYS:N	2.53	0.41
1:A:191:THR:HA	1:A:236:MET:O	2.21	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
5:A:989:HOH:O	5:A:989:HOH:O[3_555]	1.65	0.55

## 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	677/690 (98%)	630 (93%)	40 (6%)	7 (1%)	18	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	LEU
1	A	422	ASN
1	A	490	TYR
1	A	300	PHE
1	A	395	GLN
1	A	184	PRO
1	A	369	ILE

### 5.3.2 Protein sidechains [i](#)

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	606/616 (98%)	596 (98%)	10 (2%)	66	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LEU
1	A	295	LEU
1	A	372	GLU
1	A	410	ASN

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Mol	Chain	Res	Type
1	A	456	LEU
1	A	485	TYR
1	A	488	LYS
1	A	506	ASN
1	A	683	ARG
1	A	741	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	306	ASN
1	A	359	GLN
1	A	398	GLN
1	A	497	ASN
1	A	544	ASN
1	A	570	GLN
1	A	582	ASN
1	A	598	GLN
1	A	619	HIS
1	A	637	ASN
1	A	642	GLN
1	A	647	ASN
1	A	700	GLN
1	A	709	HIS
1	A	716	ASN
1	A	717	GLN
1	A	722	HIS
1	A	770	ASN

### 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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
2	ADP	A	801	4	25,29,29	1.06	2 (8%)	24,45,45	1.75	2 (8%)
3	SO4	A	802	-	4,4,4	0.45	0	6,6,6	0.10	0
3	SO4	A	803	-	4,4,4	0.43	0	6,6,6	0.19	0

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	801	4	-	0/12/32/32	0/3/3/3
3	SO4	A	802	-	-	0/0/0/0	0/0/0/0
3	SO4	A	803	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ADP	C2-N3	2.16	1.35	1.32
2	A	801	ADP	C5-C4	3.25	1.47	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	N3-C2-N1	-6.98	122.78	128.86
2	A	801	ADP	C4-C5-N7	-2.37	107.12	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	1	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 ⓘ

### 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	679/690 (98%)	0.69	82 (12%) 5 5	27, 60, 105, 126	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	PRO	8.5
1	A	376	LEU	7.5
1	A	489	ALA	6.3
1	A	385	ILE	5.9
1	A	373	VAL	5.9
1	A	371	ARG	5.5
1	A	321	ILE	5.5
1	A	378	PRO	5.4
1	A	457	LEU	5.4
1	A	297	ALA	5.2
1	A	340	ILE	5.1
1	A	383	ILE	4.9
1	A	417	VAL	4.8
1	A	490	TYR	4.7
1	A	524	HIS	4.6
1	A	492	THR	4.4
1	A	488	LYS	4.4
1	A	491	LYS	4.4
1	A	322	PHE	4.3
1	A	366	CYS	4.3
1	A	450	ARG	4.2
1	A	374	ASP	4.1
1	A	380	VAL	4.0
1	A	115	ILE	4.0
1	A	334	ALA	4.0
1	A	338	THR	3.9
1	A	386	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	367	LYS	3.7
1	A	335	ALA	3.7
1	A	296	ASP	3.7
1	A	440	GLY	3.6
1	A	487	GLU	3.5
1	A	410	ASN	3.5
1	A	411	GLY	3.5
1	A	485	TYR	3.5
1	A	493	GLU	3.4
1	A	329	ARG	3.4
1	A	452	ARG	3.3
1	A	409	GLN	3.3
1	A	379	GLU	3.3
1	A	331	TYR	3.3
1	A	368	ARG	3.3
1	A	375	ASP	3.2
1	A	369	ILE	3.2
1	A	325	PRO	3.1
1	A	495	GLN	3.1
1	A	377	GLY	3.0
1	A	356	LEU	3.0
1	A	350	GLY	2.9
1	A	337	ARG	2.9
1	A	327	PRO	2.9
1	A	323	TYR	2.8
1	A	357	THR	2.8
1	A	496	ASP	2.8
1	A	354	LEU	2.7
1	A	791	GLU	2.7
1	A	406	PRO	2.6
1	A	295	LEU	2.5
1	A	499	TYR	2.5
1	A	384	LYS	2.5
1	A	414	GLY	2.5
1	A	326	GLU	2.5
1	A	405	PRO	2.5
1	A	482	PHE	2.4
1	A	381	GLY	2.4
1	A	451	ILE	2.4
1	A	521	ASP	2.2
1	A	298	GLY	2.2
1	A	408	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	413	ILE	2.2
1	A	463	LYS	2.2
1	A	392	LEU	2.2
1	A	398	GLN	2.2
1	A	318	PRO	2.2
1	A	355	PHE	2.1
1	A	132	LYS	2.1
1	A	481	CYS	2.1
1	A	121	LEU	2.0
1	A	341	GLN	2.0
1	A	193	PRO	2.0
1	A	358	GLY	2.0
1	A	299	LYS	2.0

## 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
2	ADP	A	801	27/27	0.94	0.15	-0.26	57,77,81,84	0
4	MG	A	804	1/1	0.98	0.09	-4.53	53,53,53,53	0
3	SO4	A	803	5/5	0.92	0.25	-	80,80,82,84	0
3	SO4	A	802	5/5	0.88	0.13	-	85,96,98,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.