



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 12:50 am GMT

PDB ID : 3LC6  
Title : The alternative conformation structure of isocitrate dehydrogenase kinase/phosphatase from E. Coli  
Authors : Zheng, J.; Jia, Z.  
Deposited on : 2010-01-09  
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

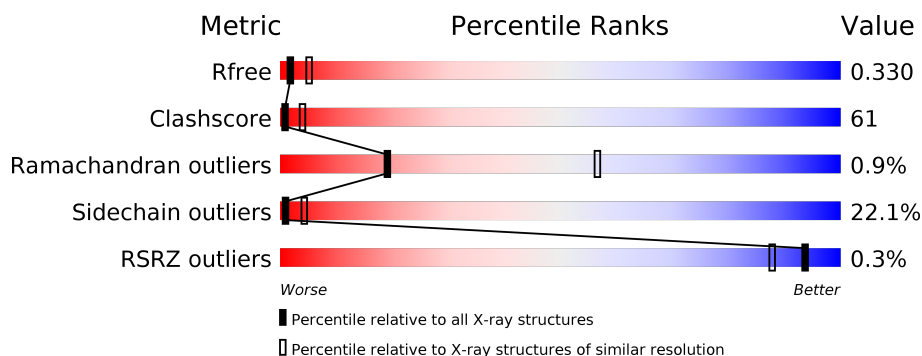
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	111664	1115 (3.12-3.08)
Clashscore	122126	1042 (3.10-3.10)
Ramachandran outliers	120053	1010 (3.10-3.10)
Sidechain outliers	120020	1010 (3.10-3.10)
RSRZ outliers	108989	1089 (3.12-3.08)

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	578	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>24%</span> <span>56%</span> <span>14%</span> <span>• 5%</span> </div> </div>
1	B	578	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>27%</span> <span>52%</span> <span>14%</span> <span>7%</span> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9107 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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4526	2906	800	799	21			
1	B	539	Total	C	N	O	S	0	0	0
			4454	2861	785	788	20			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

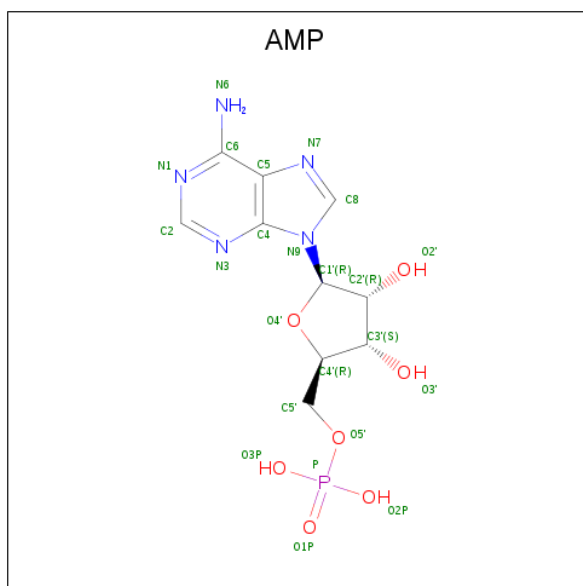


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

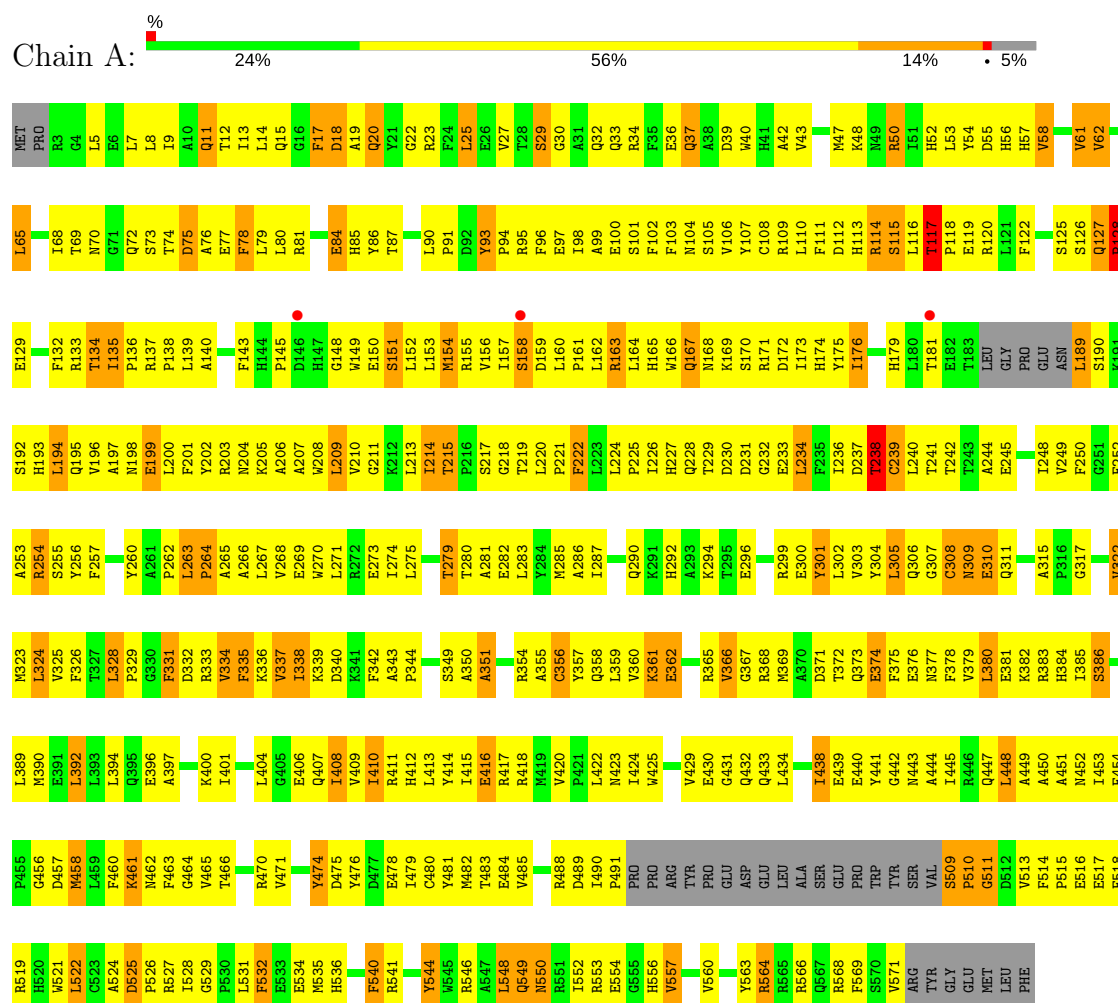
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	45	Total	O	0	0
			45	45		

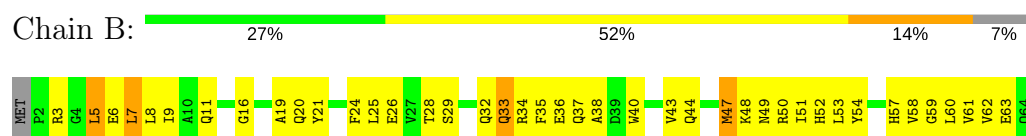
### 3 Residue-property plots

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.

- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



F518	F519	H520	W521	L522		D525		I528	G529	P530	G531	L531	F532		M535	H536	A537	D538	L539	F540	R541	D542	D543	Y544	W545	R546	A547	L548	Q549	N550	R551	I552	R553	E554	H555	Y557	E558	D559	P560	Y561	A562	Y563	R564	R565	R566	Q567	R568	F569	S570	Y571	Y573	G574	GLU	MET	LEU	PHE					
T453	F454	P455				M458	L459	F460	K461	M462	F463	G464	V465	T466	R467		R470	V471	V472	F473	Y474	D475	Y476	D477	E478	I479	G480	Y481	M482	T483	N484	V485		D489	I490	PRO	PRO	PRO	ARG	TYR	PRO	GLU	ASP	GLU	LEU	ALA	SER	GLU	PRO	TRP	TYR	SER	VAL	SER	PRO	G511	F514	P515	E516	E517	
L392	L393	L394	Q395	E396	A397	A398	E399	K400	I401	D402	D403	L404			Q407	I408	V409	I410	R411	H412	L413	Y414	I415	E416	R417	R418	M419	V420	F421	L422	N423	I424	W425	L426	E427	Q428	V429	E430	G431	Q432	Q433	L434	R435	D436	A437	I438	E439	E440	Y441	G442	M443	A444	I445	R446	Q447	L448	A449	A450	A451	N452	
F331	D332	R333	V334	F335	K336	V337	I338	K339	I340	T341	F342	ALA	PRO	GLN	LYS	GLU	MET	SER	ALA	A351	H352	V353	R354	A355	C356	Y357	Q358	L359	V360	K361	E362	H363	R364	Q365	V366	G367	R368	K369	A370	D371	T372	Q373	E374	F375	E376	N377	F378	V379	L380	E381	K382	R383	H384		P387	A388	L389	K390	E391		
V268	E269	W270	L271		I274	L275	P276	G277	T278	T279	T280	A281	E282	L283	Y284	M285	A286	I287	G288	C289	Q290	D291	H292	A293	K294	T295	E296	S297	Y298	R299	E300	Y301	Y304	L305	T306	E245	A246	S247	I311	F312	V249	F250	G251	F252	A253	R254	S255	Y256	F257	M258	V259	M321	V322	M323	L324	V325	T327	L328	P329	A266	G330
W204		W208	L209		K212	L213	I214	T215	S217	G218	T219	L220	P221	F222	L223			T226	H227	Q228	T229	D230	D231	G232	E233	L234	T236	D237	T238	C239	L240	T241	T242	T243	A244	A246	S247	I311	F312	V249	F250	G251	F252	A253	R254	S255	Y256	F257	M258	V259	M321	V322	M323	L324	V325	T327	L328	P329	A266	G330	
T134	I135	P136	R137	L138	P139	A140	K141	D142	H144	P145		W149		L152	L153	M154	R155	V156	I157	S158	D159	L160	P161	L162	R163	S101	F102		M168	K169	S170	R171	D172	H174	Y175	I176	I177	R178	H179	L180	T181		P186		L189		S192	H193	L194	Q195	V196	A197	N198	E199	L200	F201	Y202	R203			
Q72		D75		F78	L79	L80	R81	V82		H85	Y86	T87	R88	L89	L90	P91		Y92	Y93	P94	R95	F96	E97		A99	E100	S101	F102		M168	K169	S170	R171	D172	H174	Y175	I176	I177	R178	H179	L180	T181		P186		L189		S192	H193	L194	Q195	V196	A197	N198	E199	L200	F201	Y202	R203		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.14Å 133.76Å 187.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.1 (10.00-3.10) 83.7 (10.00-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	16.46 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.287 , 0.332 0.292 , 0.330	Depositor DCC
$R_{free}$ test set	1191 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 82.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	9107	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: AMP, 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	0.62	2/4643 (0.0%)	0.80	7/6283 (0.1%)
1	B	0.57	1/4567 (0.0%)	0.77	1/6179 (0.0%)
All	All	0.60	3/9210 (0.0%)	0.79	8/12462 (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	1	5
1	B	0	2
All	All	1	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	CYS	CB-SG	-6.93	1.70	1.82
1	A	511	GLY	N-CA	6.30	1.55	1.46
1	A	356	CYS	CB-SG	-5.39	1.73	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	N-CA-C	-8.62	89.69	112.10
1	A	239	CYS	N-CA-C	7.35	130.85	111.00
1	A	509	SER	N-CA-CB	-6.98	100.02	110.50
1	A	238	THR	N-CA-C	6.78	129.31	111.00
1	B	240	LEU	CA-CB-CG	6.74	130.80	115.30



All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	239	CYS	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	THR	Peptide
1	A	128	PRO	Peptide
1	A	230	ASP	Peptide
1	A	350	ALA	Peptide
1	A	510	PRO	Peptide

## 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	4526	0	4449	592	7
1	B	4454	0	4376	518	7
2	A	27	0	12	5	0
3	A	1	0	0	0	0
4	B	23	0	12	2	0
5	A	31	0	0	12	0
5	B	45	0	0	11	0
All	All	9107	0	8849	1095	7

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 61.

The worst 5 of 1095 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:279:THR:OG1	1:A:282:GLU:HG3	1.16	1.29
1:A:128:PRO:HB2	1:A:129:GLU:CA	1.56	1.29
1:A:200:LEU:HD23	1:A:201:PHE:N	1.48	1.29
1:B:550:ASN:O	1:B:554:GLU:HG3	1.31	1.29
1:A:23:ARG:O	1:A:27:VAL:HG23	1.37	1.25

The worst 5 of 7 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)
1:A:423:ASN:ND2	1:B:427:GLU:CD[2_455]	1.48	0.72
1:A:423:ASN:CG	1:B:427:GLU:OE2[2_455]	1.55	0.65
1:A:423:ASN:ND2	1:B:427:GLU:OE1[2_455]	1.74	0.46
1:A:423:ASN:ND2	1:B:427:GLU:OE2[2_455]	1.98	0.22
1:A:423:ASN:CG	1:B:427:GLU:CD[2_455]	2.01	0.19

## 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	541/578 (94%)	470 (87%)	65 (12%)	6 (1%)	16	50
1	B	529/578 (92%)	457 (86%)	68 (13%)	4 (1%)	21	59
All	All	1070/1156 (93%)	927 (87%)	133 (12%)	10 (1%)	19	56

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	232	GLY
1	A	366	VAL
1	A	511	GLY
1	B	118	PRO

### 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	480/508 (94%)	382 (80%)	98 (20%)	1	6
1	B	472/508 (93%)	360 (76%)	112 (24%)	1	3
All	All	952/1016 (94%)	742 (78%)	210 (22%)	1	4

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	GLU
1	B	112	ASP
1	B	433	GLN
1	A	564	ARG
1	B	53	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	B	32	GLN
1	B	363	HIS
1	A	536	HIS
1	B	64	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 3 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
2	ADP	A	1762	3	25,29,29	0.90	1 (4%)	25,45,45	2.14	3 (12%)
4	AMP	B	1604	-	22,25,25	1.07	1 (4%)	23,38,38	1.97	2 (8%)

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	1762	3	-	0/12/32/32	0/3/3/3
4	AMP	B	1604	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1762	ADP	C5-C4	2.57	1.46	1.40
4	B	1604	AMP	C5-C4	3.07	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1762	ADP	N3-C2-N1	-7.75	122.23	128.86
4	B	1604	AMP	N3-C2-N1	-7.22	122.69	128.86
2	A	1762	ADP	PA-O3A-PB	-4.24	118.39	132.63
4	B	1604	AMP	C4-C5-N7	-3.65	105.88	109.41
2	A	1762	ADP	C4-C5-N7	-2.93	106.58	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1762	ADP	5	0
4	B	1604	AMP	2	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	547/578 (94%)	-0.25	3 (0%) 90 81	2, 15, 29, 37	0
1	B	539/578 (93%)	-0.18	0 100 100	4, 18, 28, 34	0
All	All	1086/1156 (93%)	-0.22	3 (0%) 93 88	2, 17, 29, 37	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	THR	3.2
1	A	158	SER	2.3
1	A	146	ASP	2.3

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	AMP	B	1604	23/23	0.93	0.18	23,25,31,34	0
2	ADP	A	1762	27/27	0.95	0.15	6,10,11,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	579	1/1	0.98	0.20	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.