



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XJQ  
Title : ADP Complex OF HUMAN PAPS SYNTHETASE 1  
Authors : Harjes, S.; Bayer, P.; Scheidig, A.J.  
Deposited on : 2004-09-24  
Resolution : 2.06 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

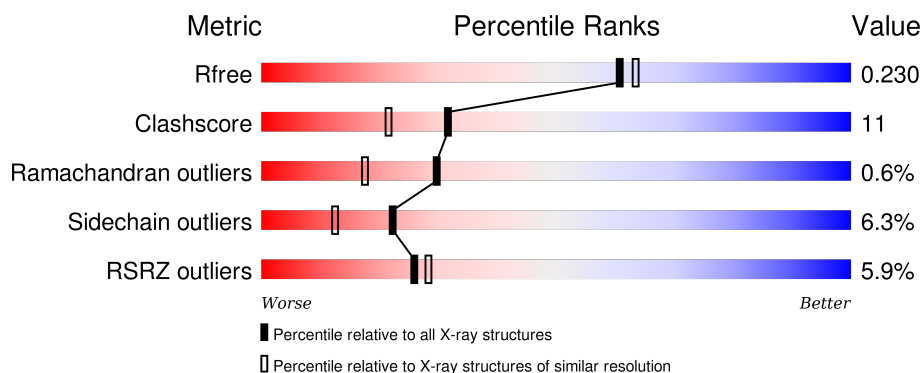
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	630	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>• • 11%</div> </div> </div>
1	B	630	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>5% • 6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9997 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 Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	590	Total	C	N	O	S	0	5	0
			4718	2990	830	867	31			
1	A	563	Total	C	N	O	S	0	8	0
			4514	2864	790	828	32			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	416	SER	PHE	CONFLICT	UNP O43252
B	625	HIS	-	EXPRESSION TAG	UNP O43252
B	626	HIS	-	EXPRESSION TAG	UNP O43252
B	627	HIS	-	EXPRESSION TAG	UNP O43252
B	628	HIS	-	EXPRESSION TAG	UNP O43252
B	629	HIS	-	EXPRESSION TAG	UNP O43252
B	630	HIS	-	EXPRESSION TAG	UNP O43252
A	416	SER	PHE	CONFLICT	UNP O43252
A	625	HIS	-	EXPRESSION TAG	UNP O43252
A	626	HIS	-	EXPRESSION TAG	UNP O43252
A	627	HIS	-	EXPRESSION TAG	UNP O43252
A	628	HIS	-	EXPRESSION TAG	UNP O43252
A	629	HIS	-	EXPRESSION TAG	UNP O43252
A	630	HIS	-	EXPRESSION TAG	UNP O43252

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

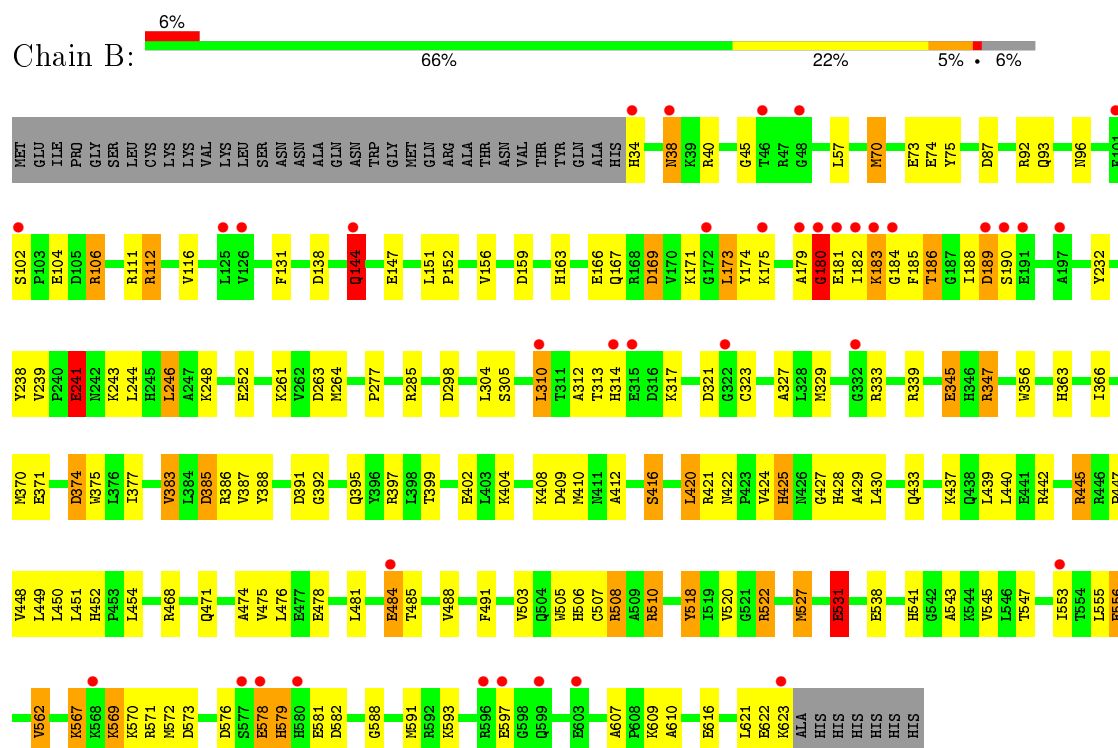
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	361	Total O 361 361	0	0
3	B	323	Total O 323 323	0	0

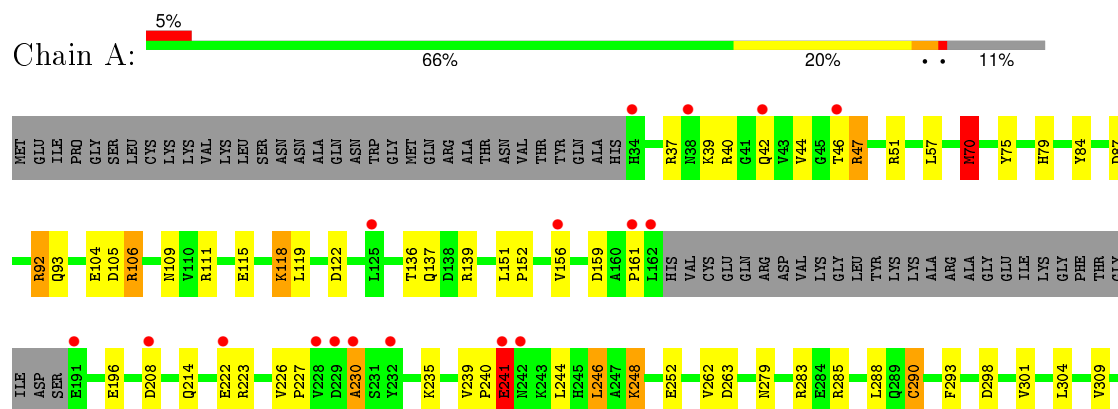
### 3 Residue-property plots

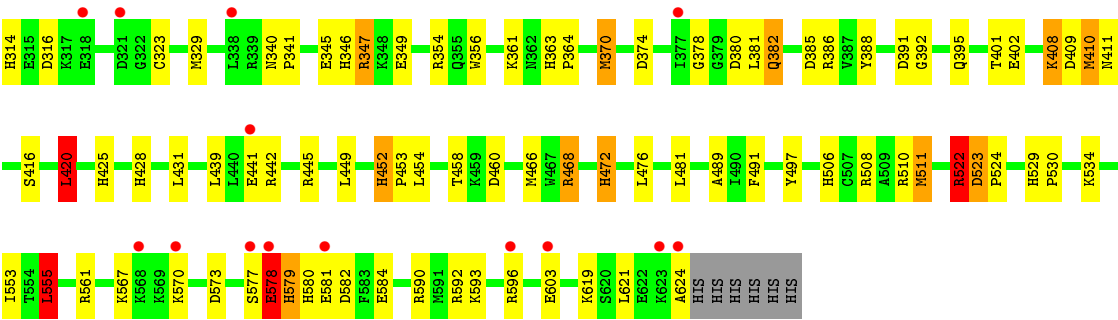
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1



- Molecule 1: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.50Å 82.50Å 133.00Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	129.10 – 2.06 19.65 – 2.06	Depositor EDS
% Data completeness (in resolution range)	96.6 (129.10-2.06) 96.7 (19.65-2.06)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.171 , 0.221 0.181 , 0.230	Depositor DCC
$R_{free}$ test set	4869 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.7	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 97370 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: 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	1.54	31/4657 (0.7%)	1.32	56/6314 (0.9%)
1	B	1.55	40/4854 (0.8%)	1.31	42/6574 (0.6%)
All	All	1.54	71/9511 (0.7%)	1.31	98/12888 (0.8%)

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	2
1	B	0	2
All	All	0	4

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ARG	CG-CD	8.74	1.73	1.51
1	B	147	GLU	CD-OE2	8.64	1.35	1.25
1	A	346	HIS	C-O	8.42	1.39	1.23
1	B	518	TYR	CE2-CZ	-7.94	1.28	1.38
1	A	402	GLU	CD-OE2	7.82	1.34	1.25

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	B	409	ASP	CB-CG-OD2	11.11	128.30	118.30
1	B	347	ARG	NE-CZ-NH2	-10.41	115.10	120.30
1	B	576	ASP	CB-CG-OD2	10.36	127.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	ASP	CB-CG-OD2	10.02	127.32	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	PRO	Peptide
1	A	230	ALA	Peptide
1	B	102	SER	Peptide
1	B	180	GLY	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	4514	0	4448	89	0
1	B	4718	0	4650	107	0
2	A	27	0	12	0	0
2	B	54	0	23	6	0
3	A	361	0	0	24	1
3	B	323	0	0	38	1
All	All	9997	0	9133	197	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 11.

The worst 5 of 197 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:591:MET:CE	1:B:591:MET:SD	2.02	1.47
1:A:70:MET:CE	1:A:70:MET:SD	2.05	1.45
1:B:70:MET:CE	1:B:70:MET:SD	2.08	1.39
1:B:527:MET:SD	1:B:527:MET:CE	2.09	1.39
1:A:370:MET:CE	1:A:370:MET:SD	2.18	1.31

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1218:HOH:O	3:A:1007:HOH:O[1_455]	2.00	0.20

## 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	566/630 (90%)	551 (97%)	14 (2%)	1 (0%)	52 43
1	B	592/630 (94%)	567 (96%)	19 (3%)	6 (1%)	19 8
All	All	1158/1260 (92%)	1118 (96%)	33 (3%)	7 (1%)	30 17

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	GLY
1	B	183	LYS
1	B	579	HIS
1	A	579	HIS
1	B	597	GLU

### 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	489/538 (91%)	460 (94%)	29 (6%)	24 14
1	B	508/538 (94%)	472 (93%)	36 (7%)	18 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	997/1076 (93%)	932 (94%)	65 (6%)	22	12

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	570	LYS
1	A	42	GLN
1	A	577	SER
1	B	578	GLU
1	B	621	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	506	HIS
1	B	541	HIS
1	A	279	ASN
1	B	428	HIS
1	A	140	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

3 ligands are modelled in this entry.

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	900	-	22,29,29	1.54	4 (18%)	27,45,45	2.79	9 (33%)
2	ADP	B	800	-	22,29,29	1.61	5 (22%)	27,45,45	1.90	4 (14%)
2	ADP	B	900	-	22,29,29	1.86	5 (22%)	27,45,45	3.65	13 (48%)

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	900	-	-	0/12/32/32	0/3/3/3
2	ADP	B	800	-	-	0/12/32/32	0/3/3/3
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	ADP	O5'-C5'	-4.17	1.27	1.44
2	B	900	ADP	PB-O3B	-3.95	1.40	1.54
2	B	800	ADP	O2'-C2'	-2.96	1.35	1.43
2	B	900	ADP	O4'-C4'	-2.79	1.38	1.45
2	A	900	ADP	O2'-C2'	-2.53	1.36	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	ADP	N3-C2-N1	-11.48	120.10	128.89
2	A	900	ADP	N3-C2-N1	-10.34	120.97	128.89
2	B	800	ADP	N3-C2-N1	-6.88	123.63	128.89
2	B	900	ADP	O4'-C4'-C5'	-6.35	86.60	109.32
2	B	900	ADP	O2B-PB-O1B	-4.34	96.61	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	ADP	6	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	563/630 (89%)	0.16	31 (5%)	29 31	22, 37, 67, 90	3 (0%)
1	B	590/630 (93%)	0.26	37 (6%)	23 25	23, 39, 72, 104	0
All	All	1153/1260 (91%)	0.21	68 (5%)	26 28	22, 38, 69, 104	3 (0%)

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	GLU	7.0
1	A	624	ALA	6.3
1	B	184	GLY	5.5
1	B	180	GLY	4.8
1	B	179	ALA	4.7

### 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	B	900	27/27	0.98	0.07	-1.40	33,38,46,48	0
2	ADP	A	900	27/27	0.99	0.07	-1.55	30,33,39,41	0
2	ADP	B	800	27/27	0.98	0.07	-1.61	37,41,43,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.