



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:43 pm GMT

PDB ID : 3ZQ6  
Title : ADP-ALF4 COMPLEX OF M. THERM. TRC40  
Authors : Sherrill, J.; Mariappan, M.; Dominik, P.; Hegde, R.S.; Keenan, R.J.  
Deposited on : 2011-06-08  
Resolution : 2.11 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

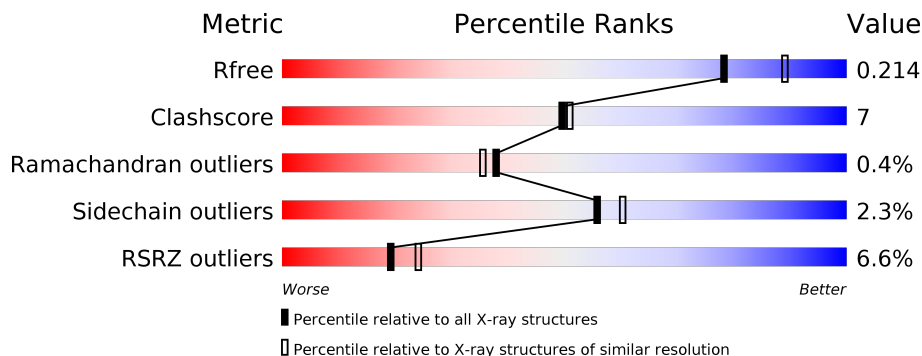
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	324	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>• 7%</div> </div> </div>
1	B	324	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>• 11%</div> </div> </div>
1	C	324	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>12%</div> </div> </div>
1	D	324	<div> <div>13%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition [i](#)

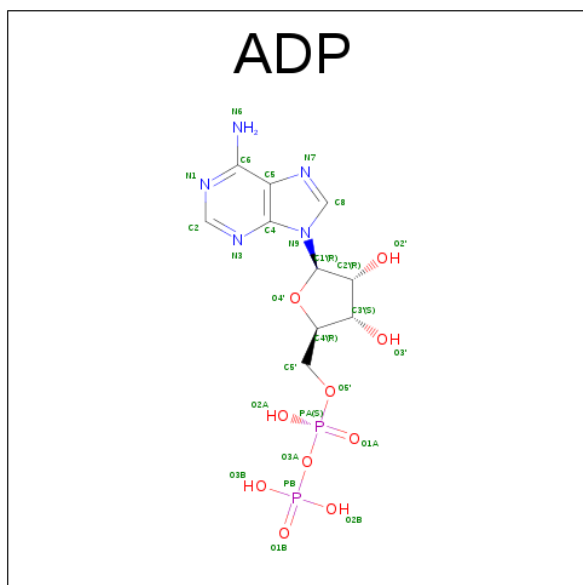
There are 7 unique types of molecules in this entry. The entry contains 9917 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PUTATIVE ARSENICAL PUMP-DRIVING ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2372	1501	395	461	15			
1	B	288	Total	C	N	O	S	0	0	0
			2274	1435	379	444	16			
1	C	284	Total	C	N	O	S	0	0	0
			2248	1417	375	442	14			
1	D	307	Total	C	N	O	S	0	0	0
			2429	1535	404	472	18			

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



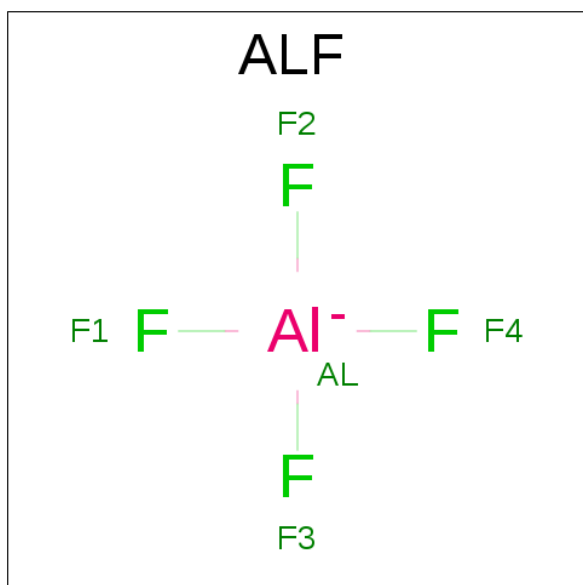
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		
3	B	1	Total	Al	F	0	0
			5	1	4		
3	C	1	Total	Al	F	0	0
			5	1	4		
3	D	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula:  $\text{Mg}$ ).

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

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	K 1	0	0
5	A	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0
5	C	1	Total 1	K 1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Zn 1	0	0
6	D	1	Total 1	Zn 1	0	0

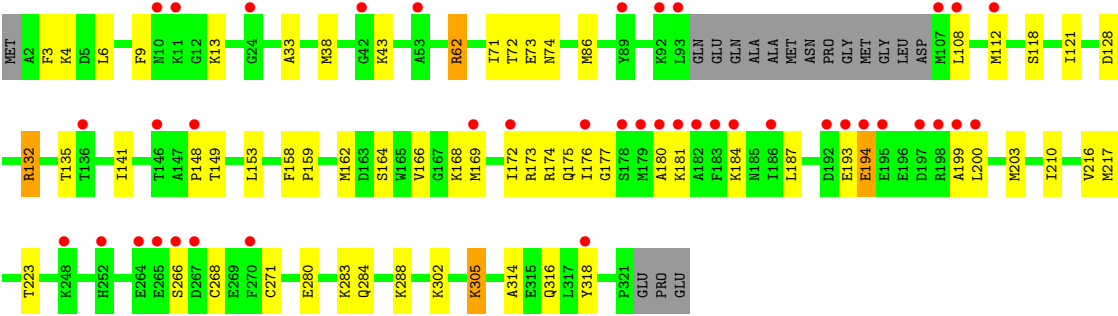
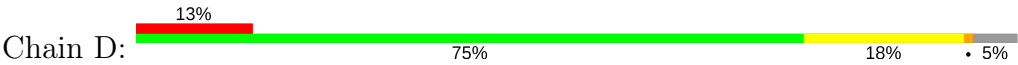
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	216	Total 216	O 216	0	0
7	B	119	Total 119	O 119	0	0
7	C	84	Total 84	O 84	0	0
7	D	37	Total 37	O 37	0	0



• Molecule 1: PUTATIVE ARSENICAL PUMP-DRIVING ATPASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.95Å 49.77Å 147.36Å 90.00° 115.04° 90.00°	Depositor
Resolution (Å)	41.21 – 2.11 41.21 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.21-2.11) 97.5 (41.21-2.11)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.173 , 0.221 0.166 , 0.214	Depositor DCC
$R_{free}$ test set	3879 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, ZN, MG, K, 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	0.55	1/2411 (0.0%)	0.62	0/3240
1	B	0.52	0/2309	0.61	0/3102
1	C	0.38	0/2283	0.53	0/3068
1	D	0.34	0/2468	0.51	0/3315
All	All	0.46	1/9471 (0.0%)	0.57	0/12725

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	CYS	CB-SG	-5.24	1.73	1.81

There are no bond angle outliers.

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	2372	0	2379	26	0
1	B	2274	0	2278	33	0
1	C	2248	0	2243	32	0
1	D	2429	0	2435	43	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	216	0	0	5	0
7	B	119	0	0	3	0
7	C	84	0	0	2	0
7	D	37	0	0	2	0
All	All	9917	0	9383	126	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 7.

The worst 5 of 126 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:305:LYS:NZ	7:A:2040:HOH:O	1.99	0.95
1:A:264:GLU:O	1:A:266:SER:N	2.15	0.79
1:B:243:MET:SD	1:B:292:LYS:HE2	2.25	0.76
1:A:88:GLU:O	1:A:92:LYS:HG2	1.86	0.75
1:B:166:VAL:O	1:B:170:ILE:HG12	1.85	0.75

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	296/324 (91%)	290 (98%)	4 (1%)	2 (1%)	25	20
1	B	282/324 (87%)	268 (95%)	13 (5%)	1 (0%)	38	35
1	C	278/324 (86%)	273 (98%)	5 (2%)	0	100	100
1	D	303/324 (94%)	295 (97%)	6 (2%)	2 (1%)	25	20
All	All	1159/1296 (89%)	1126 (97%)	28 (2%)	5 (0%)	38	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	GLU
1	A	149	THR
1	B	137	ASP
1	D	149	THR
1	D	193	GLU

### 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	257/277 (93%)	251 (98%)	6 (2%)	56	60
1	B	248/277 (90%)	242 (98%)	6 (2%)	54	59
1	C	245/277 (88%)	242 (99%)	3 (1%)	75	81
1	D	264/277 (95%)	256 (97%)	8 (3%)	46	49
All	All	1014/1108 (92%)	991 (98%)	23 (2%)	56	60

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	202	ASP
1	C	164	SER
1	D	302	LYS
1	B	206	THR
1	C	192	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	401	3,4	25,29,29	1.34	4 (16%)	24,45,45	1.43	3 (12%)
3	ALF	A	402	2,5,4,7	0,4,4	0.00	-	0,6,6	0.00	-
2	ADP	B	401	3,4	25,29,29	1.09	2 (8%)	24,45,45	1.25	2 (8%)
3	ALF	B	402	2,5,4,7	0,4,4	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	C	401	3,4	25,29,29	1.25	5 (20%)	24,45,45	1.55	5 (20%)
3	ALF	C	402	2,5,4,7	0,4,4	0.00	-	0,6,6	0.00	-
2	ADP	D	401	3,4	25,29,29	1.40	5 (20%)	24,45,45	1.38	5 (20%)
3	ALF	D	402	2,5,4,7	0,4,4	0.00	-	0,6,6	0.00	-

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	401	3,4	-	0/12/32/32	0/3/3/3
3	ALF	A	402	2,5,4,7	-	0/0/0/0	0/0/0/0
2	ADP	B	401	3,4	-	0/12/32/32	0/3/3/3
3	ALF	B	402	2,5,4,7	-	0/0/0/0	0/0/0/0
2	ADP	C	401	3,4	-	0/12/32/32	0/3/3/3
3	ALF	C	402	2,5,4,7	-	0/0/0/0	0/0/0/0
2	ADP	D	401	3,4	-	0/12/32/32	0/3/3/3
3	ALF	D	402	2,5,4,7	-	0/0/0/0	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ADP	PB-O3A	-2.43	1.56	1.60
2	A	401	ADP	PA-O2A	-2.38	1.43	1.55
2	D	401	ADP	PB-O3B	-2.31	1.45	1.54
2	C	401	ADP	PB-O3B	-2.11	1.46	1.54
2	C	401	ADP	PA-O2A	-2.10	1.44	1.55

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ADP	C1'-N9-C4	-3.80	120.06	126.64
2	C	401	ADP	O2B-PB-O1B	-2.72	99.87	110.50
2	D	401	ADP	C1'-N9-C4	-2.67	122.03	126.64
2	D	401	ADP	O3A-PB-O1B	-2.24	97.69	111.44
2	C	401	ADP	O3'-C3'-C4'	-2.11	104.91	111.09

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 [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	300/324 (92%)	-0.06	9 (3%) 51 58	13, 31, 74, 108	0
1	B	288/324 (88%)	0.26	15 (5%) 28 34	13, 35, 93, 128	0
1	C	284/324 (87%)	0.06	13 (4%) 33 39	27, 46, 97, 136	0
1	D	307/324 (94%)	0.60	41 (13%) 4 5	33, 62, 107, 145	0
All	All	1179/1296 (90%)	0.22	78 (6%) 19 24	13, 44, 98, 145	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	MET	9.4
1	B	108	LEU	5.9
1	B	200	LEU	4.9
1	D	194	GLU	4.6
1	B	201	GLN	4.4

### 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
2	ADP	D	401	27/27	0.97	0.16	0.39	23,35,40,43	0
3	ALF	A	402	5/5	0.99	0.19	0.21	16,17,18,19	0
2	ADP	B	401	27/27	0.99	0.16	0.06	11,16,21,23	0
2	ADP	A	401	27/27	0.99	0.15	0.03	11,16,20,23	0
4	MG	A	403	1/1	0.99	0.17	0.00	17,17,17,17	0
5	K	B	404	1/1	1.00	0.18	-0.02	22,22,22,22	0
2	ADP	C	401	27/27	0.99	0.12	-0.05	24,35,42,45	0
3	ALF	C	402	5/5	0.99	0.17	-0.07	27,28,35,36	0
4	MG	C	403	1/1	0.98	0.13	-0.23	31,31,31,31	0
5	K	C	404	1/1	0.99	0.13	-0.26	40,40,40,40	0
3	ALF	B	402	5/5	0.99	0.19	-0.34	17,18,19,20	0
3	ALF	D	402	5/5	0.99	0.18	-0.56	33,33,36,42	0
4	MG	B	403	1/1	0.99	0.18	-0.77	17,17,17,17	0
4	MG	D	403	1/1	0.95	0.14	-1.29	33,33,33,33	0
5	K	A	404	1/1	0.99	0.13	-1.37	23,23,23,23	0
6	ZN	D	1322	1/1	0.96	0.05	-1.69	66,66,66,66	0
6	ZN	A	1323	1/1	1.00	0.03	-1.97	49,49,49,49	0
5	K	D	404	1/1	1.00	0.14	-2.30	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.