



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID : 1K90  
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin and 3' deoxy-ATP  
Authors : Drum, C.L.; Yan, S.-Z.; Bard, J.; Shen, Y.-Q.; Lu, D.; Soelaiman, S.; Grabarek, Z.; Bohm, A.; Tang, W.-J.  
Deposited on : 2001-10-26  
Resolution : 2.75 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

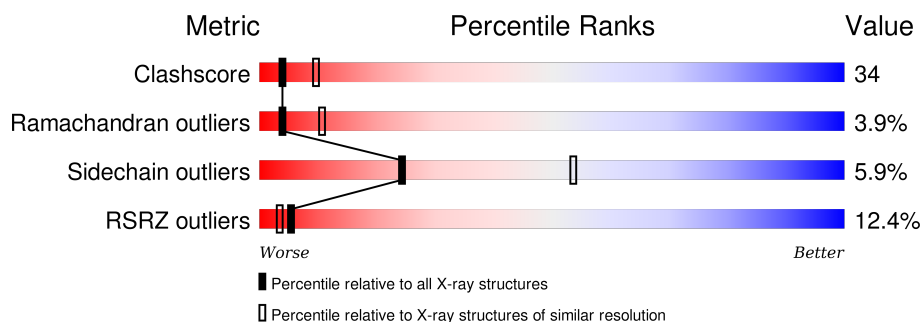
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	510	<div> <div>5%</div> <div>47%</div> <div>42%</div> <div>5%</div> <div>5%</div> </div>
1	B	510	<div> <div>12%</div> <div>35%</div> <div>48%</div> <div>8%</div> <div>9%</div> </div>
1	C	510	<div> <div>5%</div> <div>50%</div> <div>43%</div> <div>5%</div> <div>• •</div> </div>
2	D	148	<div> <div>24%</div> <div>45%</div> <div>46%</div> <div>5%</div> <div>• •</div> </div>
2	E	148	<div> <div>30%</div> <div>43%</div> <div>50%</div> <div>• •</div> <div>• •</div> </div>
2	F	148	<div> <div>26%</div> <div>41%</div> <div>51%</div> <div>• •</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15357 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 CALMODULIN-SENSITIVE ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	65	0	0
			3952	2528	673	748	3			
1	B	465	Total	C	N	O	S	113	0	0
			3794	2431	642	718	3			
1	C	503	Total	C	N	O	S	166	0	0
			4094	2616	696	779	3			

- Molecule 2 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		

- Molecule 4 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

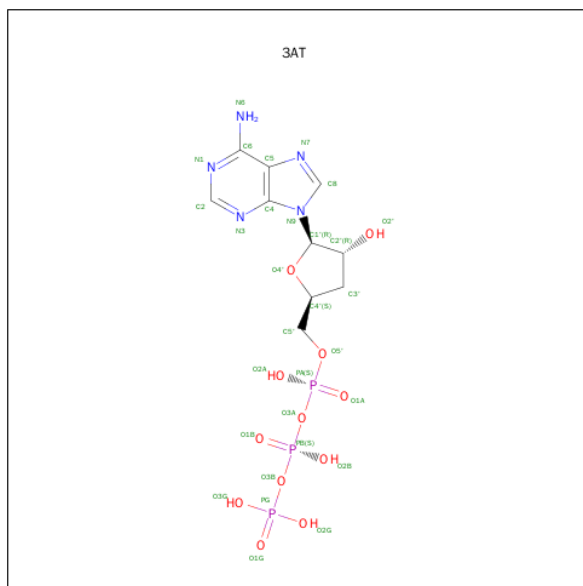
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Yb	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Yb	0	0
			1	1		
4	C	1	Total	Yb	0	0
			1	1		

- Molecule 5 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	B	8	Total	O	0	0
			8	8		
6	C	22	Total	O	0	0
			22	22		
6	D	1	Total	O	0	0
			1	1		

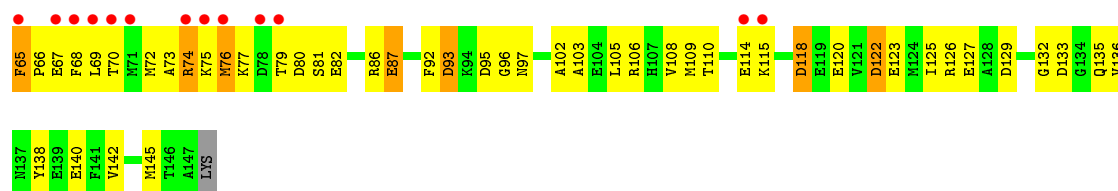
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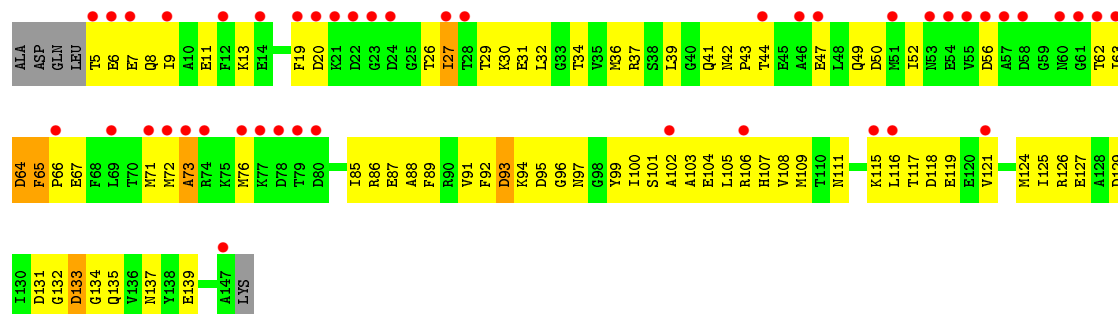
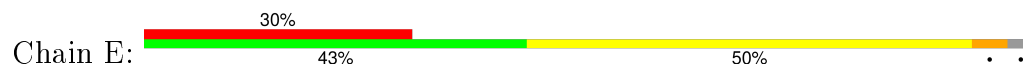
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	2	Total	O	0	0
			2	2		



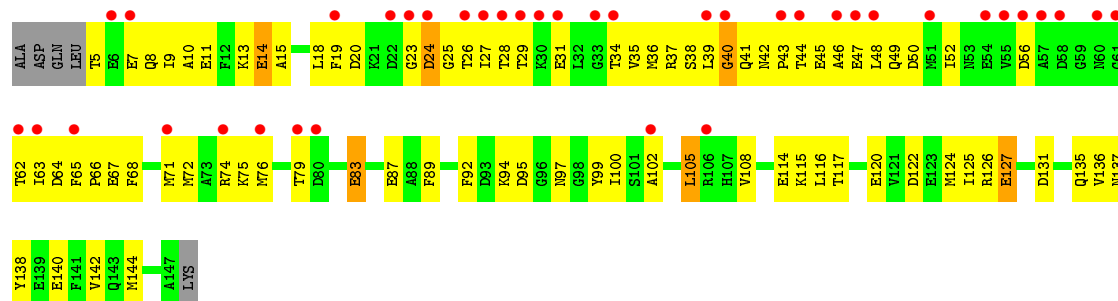
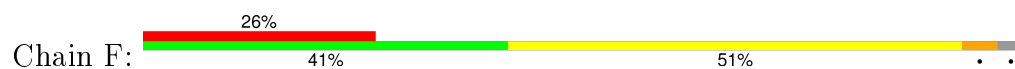




• Molecule 2: CALMODULIN



• Molecule 2: CALMODULIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.10Å 166.10Å 343.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.75 29.90 – 2.64	Depositor EDS
% Data completeness (in resolution range)	90.7 (19.97-2.75) 95.5 (29.90-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.64Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.215 , 0.286 0.251 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	66.7	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 71.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 93302 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, YB, 3AT

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	0.31	0/4027	0.59	1/5419 (0.0%)
1	B	0.30	0/3867	0.57	1/5204 (0.0%)
1	C	0.32	0/4172	0.56	1/5613 (0.0%)
2	D	0.29	0/1137	0.47	0/1527
2	E	0.26	0/1137	0.45	0/1527
2	F	0.30	0/1137	0.49	1/1527 (0.1%)
All	All	0.30	0/15477	0.55	4/20817 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	SER	N-CA-C	-10.34	83.07	111.00
1	B	743	PRO	N-CA-C	5.65	126.80	112.10
1	C	745	TYR	N-CA-C	-5.50	96.14	111.00
2	F	40	GLY	N-CA-C	5.08	125.81	113.10

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	3952	0	3999	257	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3794	0	3828	325	0
1	C	4094	0	4134	248	0
2	D	1125	0	1049	64	0
2	E	1125	0	1049	89	0
2	F	1125	0	1049	86	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	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
5	A	30	0	12	2	0
5	B	30	0	12	1	0
5	C	30	0	12	0	0
6	A	10	0	0	0	0
6	B	8	0	0	1	0
6	C	22	0	0	1	0
6	D	1	0	0	0	0
6	F	2	0	0	0	0
All	All	15357	0	15144	1026	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 34.

The worst 5 of 1026 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:616:GLU:HA	1:B:620:THR:HG22	1.37	1.06
1:B:489:THR:HG22	1:B:490:ALA:H	1.21	1.03
1:B:325:TYR:HB2	1:B:498:ALA:HB3	1.37	1.03
1:C:659:THR:HG22	1:C:661:ALA:H	1.21	1.03
1:A:783:THR:HB	1:A:789:ASN:HD21	1.30	0.96

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	479/510 (94%)	411 (86%)	52 (11%)	16 (3%)	5	14
1	B	457/510 (90%)	364 (80%)	66 (14%)	27 (6%)	2	4
1	C	499/510 (98%)	423 (85%)	60 (12%)	16 (3%)	5	15
2	D	141/148 (95%)	111 (79%)	24 (17%)	6 (4%)	3	9
2	E	141/148 (95%)	107 (76%)	29 (21%)	5 (4%)	4	13
2	F	141/148 (95%)	116 (82%)	23 (16%)	2 (1%)	14	38
All	All	1858/1974 (94%)	1532 (82%)	254 (14%)	72 (4%)	4	11

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	739	LYS
2	D	64	ASP
1	B	466	GLY
2	E	73	ALA

### 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	433/455 (95%)	410 (95%)	23 (5%)	28	58
1	B	414/455 (91%)	382 (92%)	32 (8%)	16	38
1	C	448/455 (98%)	421 (94%)	27 (6%)	24	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	121/126 (96%)	115 (95%)	6 (5%)	30	61
2	E	121/126 (96%)	117 (97%)	4 (3%)	45	77
2	F	121/126 (96%)	115 (95%)	6 (5%)	30	61
All	All	1658/1743 (95%)	1560 (94%)	98 (6%)	24	53

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	545	THR
1	B	714	GLN
1	C	775	LEU
1	B	546	LYS
1	B	620	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	518	ASN
1	B	730	ASN
1	C	734	ASN
1	B	526	GLN
1	B	629	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 12 ligands modelled in this entry, 9 are 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$
5	3AT	A	902	4	24,32,32	1.38	4 (16%)	26,50,50	1.24	1 (3%)
5	3AT	B	903	4	24,32,32	1.38	5 (20%)	26,50,50	1.25	2 (7%)
5	3AT	C	904	4	24,32,32	1.41	6 (25%)	26,50,50	1.21	1 (3%)

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
5	3AT	A	902	4	-	0/18/34/34	0/3/3/3
5	3AT	B	903	4	-	0/18/34/34	0/3/3/3
5	3AT	C	904	4	-	0/18/34/34	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	902	3AT	PG-O2G	-3.03	1.43	1.54
5	B	903	3AT	PG-O2G	-2.60	1.45	1.54
5	C	904	3AT	PG-O3G	-2.49	1.45	1.54
5	C	904	3AT	PB-O2B	-2.42	1.44	1.54
5	C	904	3AT	PG-O2G	-2.38	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	903	3AT	C4-C5-N7	2.16	111.46	109.48
5	A	902	3AT	O3G-PG-O2G	2.62	117.38	107.38
5	B	903	3AT	O3G-PG-O2G	2.66	117.51	107.38
5	C	904	3AT	O3G-PG-O2G	2.70	117.65	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	902	3AT	2	0
5	B	903	3AT	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 [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	485/510 (95%)	0.07	26 (5%)	29 22	24, 64, 145, 174	16 (3%)
1	B	457/510 (89%)	0.58	60 (13%)	5 3	29, 79, 172, 191	12 (2%)
1	C	491/510 (96%)	0.13	25 (5%)	32 24	17, 62, 151, 177	19 (3%)
2	D	143/148 (96%)	1.18	35 (24%)	1 0	39, 134, 185, 193	0
2	E	143/148 (96%)	1.72	45 (31%)	1 0	61, 159, 199, 199	0
2	F	143/148 (96%)	1.23	39 (27%)	1 0	43, 145, 188, 198	0
All	All	1862/1974 (94%)	0.51	230 (12%)	5 3	17, 76, 181, 199	47 (2%)

The worst 5 of 230 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	19	PHE	17.2
2	D	57	ALA	12.5
2	E	62	THR	10.9
1	B	697	ILE	10.7
2	F	62	THR	10.6

### 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(Å <sup>2</sup> )	Q<0.9
3	CA	F	804	1/1	0.98	0.16	0.55	67,67,67,67	0
5	3AT	A	902	30/30	0.96	0.20	0.40	23,44,55,55	0
5	3AT	B	903	30/30	0.96	0.22	-0.02	43,54,61,65	0
5	3AT	C	904	30/30	0.96	0.17	-0.27	28,44,53,58	0
3	CA	D	801	1/1	0.96	0.12	-0.38	59,59,59,59	0
3	CA	D	800	1/1	0.97	0.14	-1.02	53,53,53,53	0
3	CA	E	802	1/1	0.96	0.13	-1.27	105,105,105,105	0
3	CA	E	803	1/1	0.96	0.07	-1.41	83,83,83,83	0
3	CA	F	805	1/1	0.98	0.05	-4.09	63,63,63,63	0
4	YB	B	902	1/1	0.99	0.18	-	47,47,47,47	0
4	YB	C	903	1/1	0.99	0.17	-	38,38,38,38	0
4	YB	A	901	1/1	1.00	0.18	-	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.