

# wwPDB X-ray Structure Validation Summary Report (i)

#### Feb 10, 2024 – 04:38 PM EST

PDB ID : 2QRE

Title : Crystal structure of the adenylate sensor from AMP-activated protein kinase

in complex with 5-aminoimidazole-4-carboxamide 1-beta-D-ribofuranotide

(ZMP)

Authors : Jin, X.; Townley, R.; Shapiro, L.

Deposited on : 2007-07-28

Resolution : 3.01 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

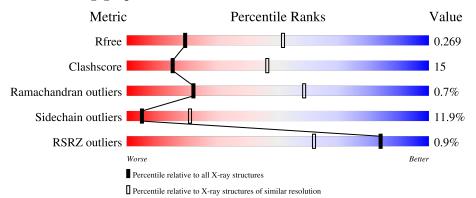
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 3.01 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	137	47%	28% • • 20%	_
1	С	137	55%	23% • 18%	
2	В	97	55%	27% 6% 12%	6
2	D	97	57%	32% 5%	6%



 $Continued\ from\ previous\ page...$ 

Mol	Chain	Length	Quality of o	chain	
3	Е	334	56%	34%	• 6%
3	G	334	63%	25%	6% 6%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8201 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 SNF1-like protein kinase ssp2.

	$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
Ī	1	Λ	109	Total	С	N	О	S	0	0	0
	1	1 A	109	882	572	148	153	9	U	U	
	1	С	113	Total	С	N	О	S	0	0	0
	1	C	110	903	583	155	156	9	U		

• Molecule 2 is a protein called SPCC1919.03c protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	85	Total 668		N 115	O 123	S 2	0	0	0
2	D	91	Total 718			O 134	S 2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	202	MET	-	expression tag	UNP P78789
D	202	MET	-	expression tag	UNP P78789

• Molecule 3 is a protein called Protein C1556.08c.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
3	G	315	Total 2478	C 1585	- 1	O 464	S 15	0	0	0
3	Е	315	Total 2489	C 1591	- '	O 466	S 15	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

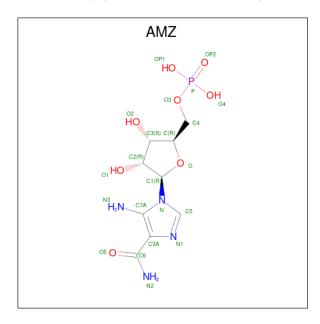
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	expression tag	UNP Q10343
G	2	MET	-	expression tag	UNP Q10343



 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ALA	-	expression tag	UNP Q10343
E	2	MET	-	expression tag	UNP Q10343

• Molecule 4 is AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (three-letter code: AMZ) (formula:  $C_9H_{15}N_4O_8P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
4	G	1	Total 22		N 4		P	0	0	
4	I.	1	Total	-			P	0	0	
4	4 E	1	22	9	4	8	1	U	U	

• Molecule 5 is water.

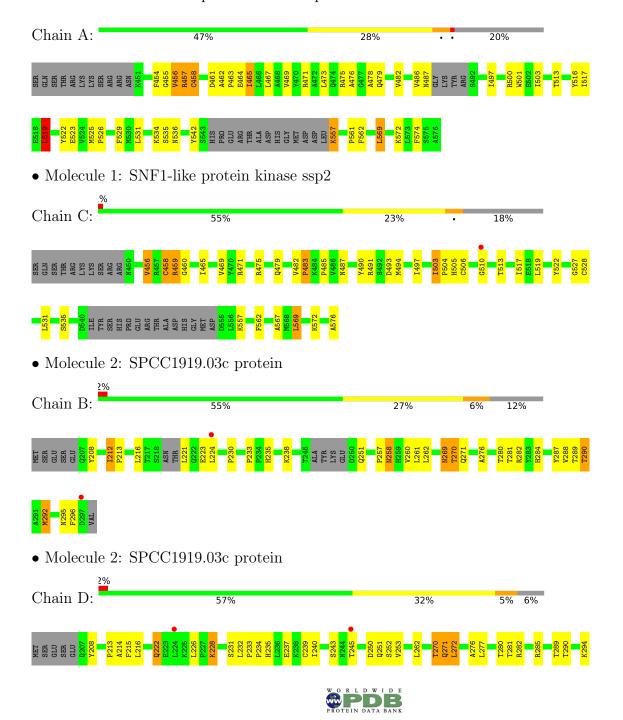
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	В	1	Total O 1 1	0	0
5	G	9	Total O 9 9	0	0
5	С	2	Total O 2 2	0	0
5	D	2	Total O 2 2	0	0
5	E	4	Total O 4 4	0	0



## 3 Residue-property plots (i)

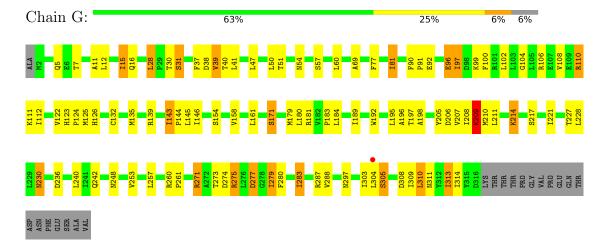
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SNF1-like protein kinase ssp2

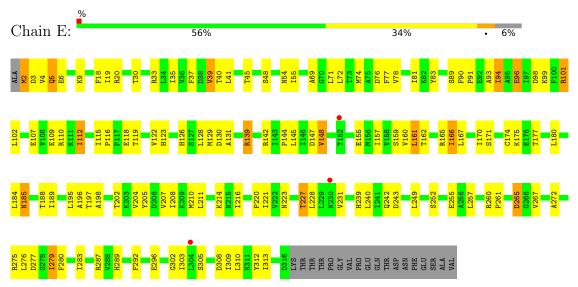




• Molecule 3: Protein C1556.08c



• Molecule 3: Protein C1556.08c





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	168.47Å 78.15Å 108.51Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 124.04° 90.00°	Depositor
Resolution (Å)	41.34 - 3.01	Depositor
Resolution (A)	41.34 - 3.01	EDS
% Data completeness	89.2 (41.34-3.01)	Depositor
(in resolution range)	89.2 (41.34-3.01)	EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.32 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.235 , 0.297	Depositor
$R, R_{free}$	0.247 , $0.269$	DCC
$R_{free}$ test set	1074 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.28 , 86.0	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	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>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: AMZ

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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.58	0/904	0.70	2/1215~(0.2%)
1	С	0.55	0/926	0.63	0/1246
2	В	0.49	0/683	0.85	4/931~(0.4%)
2	D	0.49	0/736	0.75	1/1006~(0.1%)
3	Е	0.53	0/2534	0.68	0/3433
3	G	0.52	0/2520	0.69	2/3415~(0.1%)
All	All	0.53	0/8303	0.70	9/11246 (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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	Ε	0	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
2	В	258	ASN	CB-CA-C	6.89	124.17	110.40
2	В	224	LEU	N-CA-C	-6.25	94.13	111.00
2	В	223	GLU	N-CA-C	6.10	127.48	111.00
1	A	519	LEU	CA-CB-CG	5.86	128.79	115.30
2	В	223	GLU	CB-CA-C	-5.77	98.86	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	Е	2	MET	Peptide
3	G	209	LYS	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	882	0	880	33	0
1	С	903	0	889	23	0
2	В	668	0	676	23	0
2	D	718	0	724	22	0
3	Е	2489	0	2545	90	0
3	G	2478	0	2530	81	0
4	Е	22	0	13	1	0
4	G	22	0	13	2	0
5	A	1	0	0	0	0
5	В	1	0	0	0	0
5	С	2	0	0	0	0
5	D	2	0	0	0	0
5	Е	4	0	0	0	0
5	G	9	0	0	0	0
All	All	8201	0	8270	246	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 15.

The worst 5 of 246 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
3:G:81:ILE:HD11	3:G:208:ILE:CD1	1.41	1.47
3:G:81:ILE:CD1	3:G:208:ILE:CD1	2.22	1.18
3:G:81:ILE:CD1	3:G:208:ILE:HD11	1.72	1.16
3:E:3:ASP:O	3:E:4:VAL:HG12	1.57	1.03
3:G:208:ILE:HA	3:G:211:LEU:HD12	1.41	1.02

There are no symmetry-related clashes.



### 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	Perce	entiles
1	A	103/137 (75%)	97 (94%)	5 (5%)	1 (1%)	15	50
1	С	109/137 (80%)	102 (94%)	5 (5%)	2 (2%)	8	35
2	В	79/97 (81%)	73 (92%)	6 (8%)	0	100	100
2	D	89/97 (92%)	74 (83%)	13 (15%)	2 (2%)	6	30
3	E	314/334 (94%)	284 (90%)	29 (9%)	1 (0%)	41	75
3	G	313/334 (94%)	291 (93%)	21 (7%)	1 (0%)	41	75
All	All	1007/1136 (89%)	921 (92%)	79 (8%)	7 (1%)	22	59

#### 5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	510	GLY
1	A	455	GLY
3	G	135	MET
2	D	215	PHE
2	D	243	SER

#### 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	95/120~(79%)	85 (90%)	10 (10%)	7 26
1	С	94/120 (78%)	86 (92%)	8 (8%)	10 36
2	В	77/88 (88%)	69 (90%)	8 (10%)	7 26



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Per	centiles
2	D	82/88 (93%)	70 (85%)	12 (15%)	3	14
3	E	280/296~(95%)	244 (87%)	36 (13%)	4	18
3	G	278/296 (94%)	244 (88%)	34 (12%)	5	20
All	All	906/1008 (90%)	798 (88%)	108 (12%)	5	21

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	503	ILE
2	D	290	THR
3	Е	228	LEU
1	С	569	LEU
2	D	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	222	GLN
3	Ε	66	ASN
3	Е	242	GLN
3	Ε	123	HIS
2	D	284	HIS

#### 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 monosaccharides in this entry.



## 5.6 Ligand geometry (i)

2 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	Trunc	Chain	Res	Dag	Dag	Dec	Dec	Dag	Dag	Dag	Their Dec	Link	Bond lengths			Bond angles		
	Type			LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2								
4	AMZ	Е	1002	-	18,23,23	0.77	0	22,35,35	1.36	3 (13%)								
4	AMZ	G	1001	-	18,23,23	0.81	0	22,35,35	1.17	2 (9%)								

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.

$\mathbf{M}$	ol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4	AMZ	Е	1002	-	-	5/6/30/30	0/2/2/2
4	1	AMZ	G	1001	-	-	0/6/30/30	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
4	Е	1002	AMZ	C5-N1-C3A	2.86	108.44	102.99
4	Е	1002	AMZ	C3A-C6-N2	2.65	119.94	115.75
4	G	1001	AMZ	O4-P-OP2	2.14	119.06	110.68
4	G	1001	AMZ	O4-P-O3	-2.04	101.31	106.73
4	Е	1002	AMZ	O4-P-OP1	2.03	115.40	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Е	1002	AMZ	C4-O3-P-OP1
4	Е	1002	AMZ	C4-O3-P-O4
4	Е	1002	AMZ	C4-O3-P-OP2



Continued from previous page...

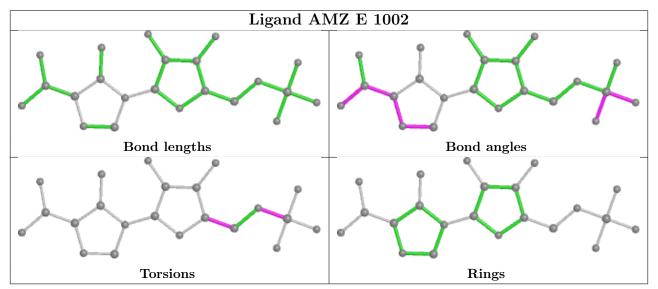
Mol	Chain	Res	Type	Atoms
4	Е	1002	AMZ	O-C-C4-O3
4	Е	1002	AMZ	C3-C-C4-O3

There are no ring outliers.

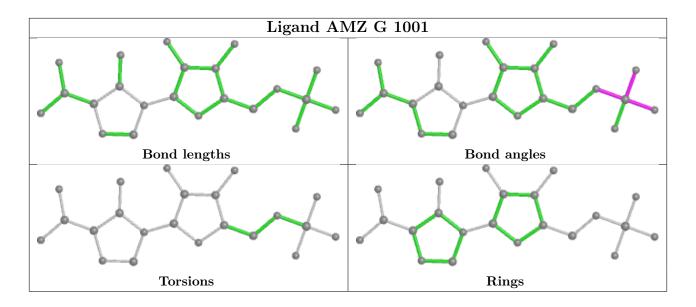
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Е	1002	AMZ	1	0
4	G	1001	AMZ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	109/137 (79%)	-0.25	0 100 100	82, 90, 94, 98	1 (0%)
1	С	113/137 (82%)	-0.15	1 (0%) 84 62	84, 90, 95, 98	0
2	В	85/97 (87%)	-0.20	2 (2%) 59 30	28, 89, 95, 99	0
2	D	91/97 (93%)	0.07	2 (2%) 62 32	28, 90, 94, 96	0
3	Е	315/334 (94%)	-0.34	3 (0%) 82 58	32, 90, 97, 104	1 (0%)
3	G	315/334 (94%)	-0.39	1 (0%) 94 83	28, 89, 97, 109	1 (0%)
All	All	1028/1136 (90%)	-0.28	9 (0%) 84 62	28, 90, 96, 109	3 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	224	LEU	3.6
3	Е	304	LEU	3.3
2	В	224	LEU	3.3
1	С	510	GLY	3.3
3	Е	152	THR	2.6

### 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 monosaccharides in this entry.

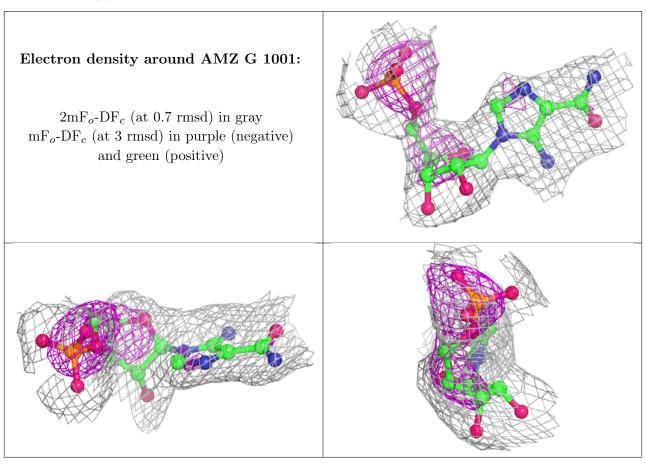


## 6.4 Ligands (i)

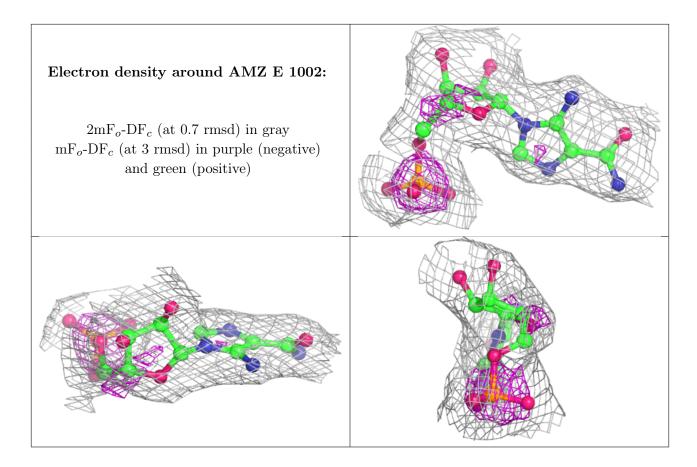
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
4	AMZ	G	1001	22/22	0.95	0.15	77,79,80,81	0
4	AMZ	Е	1002	22/22	0.96	0.14	82,85,90,90	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







## 6.5 Other polymers (i)

There are no such residues in this entry.

