



# wwPDB X-ray Structure Validation Summary Report i

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PDB ID : 1GX3  
Title : M. SMEGMATIS ARYLAMINE N-ACETYL TRANSFERASE  
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Deposited on : 2002-03-26  
Resolution : 1.70 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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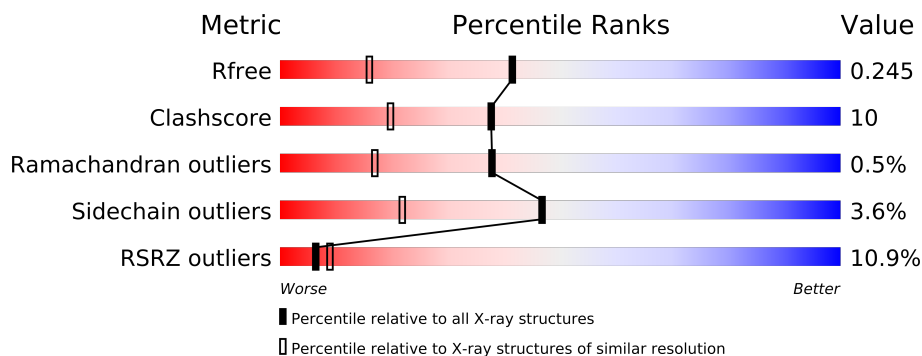
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	284	
1	B	284	
1	C	284	
1	D	284	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9263 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ARYLAMINE N-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2136	1339	395	398	4			
1	B	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			
1	C	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			
1	D	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	295	Total	O	0	0
			295	295		
2	B	218	Total	O	0	0
			218	218		
2	C	157	Total	O	0	0
			157	157		
2	D	85	Total	O	0	0
			85	85		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.25Å 105.83Å 141.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 84.71 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.70) 97.8 (84.71-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.209 , 0.241 0.216 , 0.245	Depositor DCC
$R_{free}$ test set	8181 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.7	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 163201 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9263	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

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	1.13	3/2184 (0.1%)	1.21	17/2974 (0.6%)
1	B	1.13	4/2172 (0.2%)	1.17	17/2959 (0.6%)
1	C	1.12	8/2172 (0.4%)	1.17	13/2959 (0.4%)
1	D	0.73	0/2172	0.96	12/2959 (0.4%)
All	All	1.04	15/8700 (0.2%)	1.13	59/11851 (0.5%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	GLU	CD-OE1	6.43	1.32	1.25
1	B	29	VAL	CB-CG1	6.30	1.66	1.52
1	C	29	VAL	CB-CG1	-5.98	1.40	1.52
1	C	137	SER	CA-CB	5.83	1.61	1.52
1	B	112	VAL	CB-CG2	-5.63	1.41	1.52

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	CB-CG-OD2	9.96	127.26	118.30
1	A	64	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	D	188	ASP	CB-CG-OD2	9.06	126.45	118.30
1	C	4	ASP	CB-CG-OD2	8.56	126.00	118.30
1	A	64	ARG	NE-CZ-NH1	8.53	124.57	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2136	0	0	16	1
1	B	2124	0	0	20	0
1	C	2124	0	0	25	1
1	D	2124	0	0	25	0
2	A	295	0	0	13	1
2	B	218	0	0	17	0
2	C	157	0	0	15	1
2	D	85	0	0	11	0
All	All	9263	0	0	85	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 85 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:TRP:CD2	2:A:2148:HOH:O	2.12	1.00
1:A:97:TRP:CE3	2:A:2148:HOH:O	2.12	1.00
1:A:15:ASP:OD1	2:A:2035:HOH:O	1.81	0.98
1:B:229:HIS:CD2	2:B:2194:HOH:O	2.27	0.88
1:B:186:ARG:NH1	2:B:2163:HOH:O	2.09	0.85

All (2) 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	Distance(Å)	Clash(Å)
1:A:15:ASP:OD2	1:C:34:ARG:NH1[3_545]	2.12	0.08
2:A:2029:HOH:O	2:C:2006:HOH:O[3_545]	2.19	0.01

## 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	274/284 (96%)	264 (96%)	10 (4%)	0	100	100
1	B	272/284 (96%)	261 (96%)	10 (4%)	1 (0%)	43	22
1	C	272/284 (96%)	262 (96%)	8 (3%)	2 (1%)	30	10
1	D	272/284 (96%)	246 (90%)	24 (9%)	2 (1%)	30	10
All	All	1090/1136 (96%)	1033 (95%)	52 (5%)	5 (0%)	38	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	18	PRO
1	B	3	MET
1	C	160	GLY
1	D	20	PRO
1	C	161	ASP

### 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	221/228 (97%)	214 (97%)	7 (3%)	51	26
1	B	220/228 (96%)	210 (96%)	10 (4%)	38	15
1	C	220/228 (96%)	213 (97%)	7 (3%)	51	26
1	D	220/228 (96%)	212 (96%)	8 (4%)	47	22
All	All	881/912 (97%)	849 (96%)	32 (4%)	47	22

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	229	HIS
1	C	39	GLU
1	D	224	ARG
1	B	259	ASP
1	C	65	ARG

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

such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	276/284 (97%)	0.42	6 (2%) 59 64	18, 26, 47, 68	0
1	B	274/284 (96%)	0.60	16 (5%) 22 26	20, 32, 54, 65	0
1	C	274/284 (96%)	0.61	28 (10%) 7 10	21, 35, 58, 69	0
1	D	274/284 (96%)	1.42	70 (25%) 1 2	28, 51, 73, 82	0
All	All	1098/1136 (96%)	0.76	120 (10%) 6 9	18, 35, 63, 82	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	ALA	9.2
1	D	119	GLY	7.7
1	D	3	MET	7.1
1	D	232	GLY	6.9
1	D	117	VAL	6.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.