



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:43 PM GMT

PDB ID : 1GX3
Title : M. SMEGMATIS ARYLAMINE N-ACETYL TRANSFERASE
Authors : Sandy, J.; Mushtaq, A.; Kawamura, A.; Sinclair, J.; Sim, E.; Noble, M.
Deposited on : 2002-03-26
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

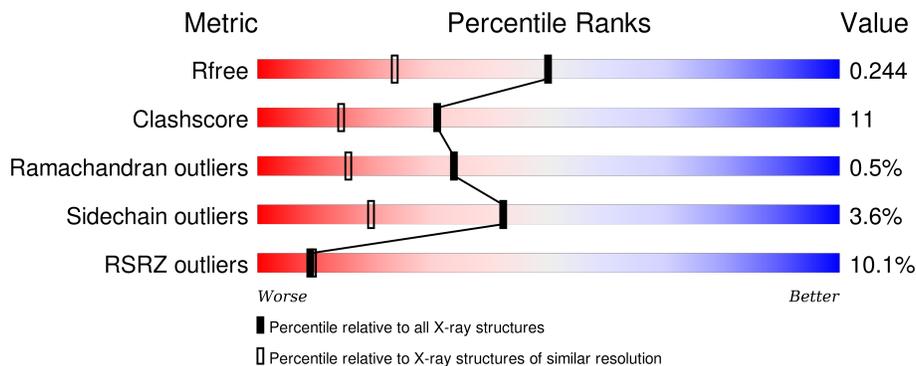
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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 ≥ 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	284	 2% 85% 10% . .
1	B	284	 6% 75% 19% . . .
1	C	284	 9% 74% 18% . .
1	D	284	 23% 68% 25% . .

2 Entry composition

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

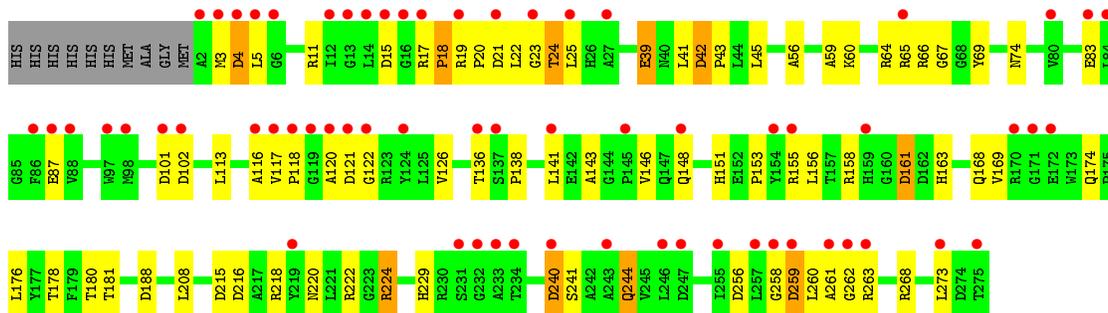
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ARYLAMINE N-ACETYLTRANSFERASE.

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

- Molecule 2 is water.

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.70Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.241 0.215 , 0.244	Depositor DCC
R_{free} test set	8179 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	28.1	Xtrriage
Anisotropy	0.559	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 163201 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9263	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage'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.*

¹ Intensities estimated from amplitudes.

² 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 [\(i\)](#)

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 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	2136	0	2095	27	1
1	B	2124	0	2080	42	0
1	C	2124	0	2080	54	1
1	D	2124	0	2080	62	0
2	A	295	0	0	16	1
2	B	218	0	0	21	0
2	C	157	0	0	13	1
2	D	85	0	0	12	0
All	All	9263	0	8335	183	2

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 183 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:15:ASP:HB2	2:A:2034:HOH:O	1.53	1.08
1:B:259:ASP:HB2	2:B:2205:HOH:O	1.61	1.01
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:D:241:SER:H	1:D:244:GLN:HE22	1.08	0.99

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	Interatomic distance (Å)	Clash overlap (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 [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	274/284 (96%)	264 (96%)	10 (4%)	0	100	100
1	B	272/284 (96%)	261 (96%)	10 (4%)	1 (0%)	39	20
1	C	272/284 (96%)	262 (96%)	8 (3%)	2 (1%)	26	9
1	D	272/284 (96%)	246 (90%)	24 (9%)	2 (1%)	26	9
All	All	1090/1136 (96%)	1033 (95%)	52 (5%)	5 (0%)	34	15

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 [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	221/228 (97%)	214 (97%)	7 (3%)	46	24
1	B	220/228 (96%)	210 (96%)	10 (4%)	34	13
1	C	220/228 (96%)	213 (97%)	7 (3%)	46	24
1	D	220/228 (96%)	212 (96%)	8 (4%)	42	19
All	All	881/912 (97%)	849 (96%)	32 (4%)	42	19

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

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Mol	Chain	Res	Type
1	C	65	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	GLN
1	C	33	ASN
1	D	174	GLN
1	B	244	GLN
1	B	251	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](#)

There are no ligands in this entry.

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, 95th 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 ²)	Q < 0.9
1	A	276/284 (97%)	0.39	6 (2%) 65 70	18, 26, 47, 68	0
1	B	274/284 (96%)	0.51	16 (5%) 26 28	20, 32, 54, 65	0
1	C	274/284 (96%)	0.59	25 (9%) 11 13	21, 35, 58, 69	0
1	D	274/284 (96%)	1.24	64 (23%) 1 1	28, 51, 73, 82	0
All	All	1098/1136 (96%)	0.68	111 (10%) 9 9	18, 35, 63, 82	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.5
1	D	119	GLY	7.4
1	D	233	ALA	7.2
1	D	3	MET	7.2
1	D	117	VAL	6.8

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](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.