



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:48 pm GMT

PDB ID : 2BSZ  
Title : Structure of Mesorhizobium loti arylamine N-acetyltransferase 1  
Authors : Holton, S.J.; Dairou, J.; Sandy, J.; Rodrigues-Lima, F.; Dupret, J.-M.; Noble, M.E.M.; Sim, E.  
Deposited on : 2005-05-24  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
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

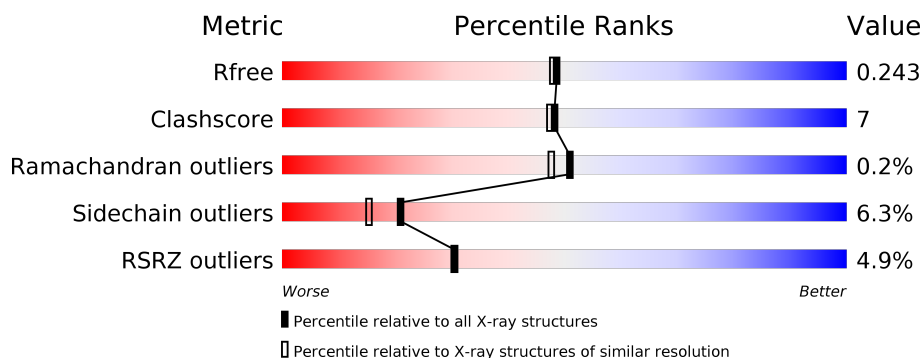
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 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	278	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	278	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4430 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2099	1341	372	383	3			
1	B	264	Total	C	N	O	S	0	0	0
			2075	1325	369	378	3			

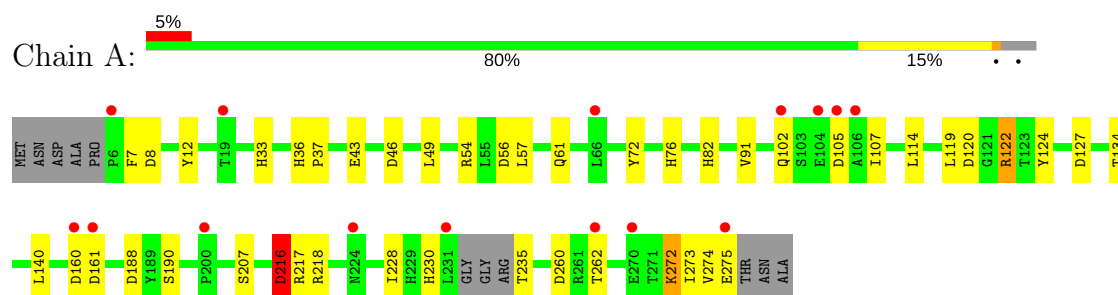
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		
2	B	117	Total	O	0	0
			117	117		

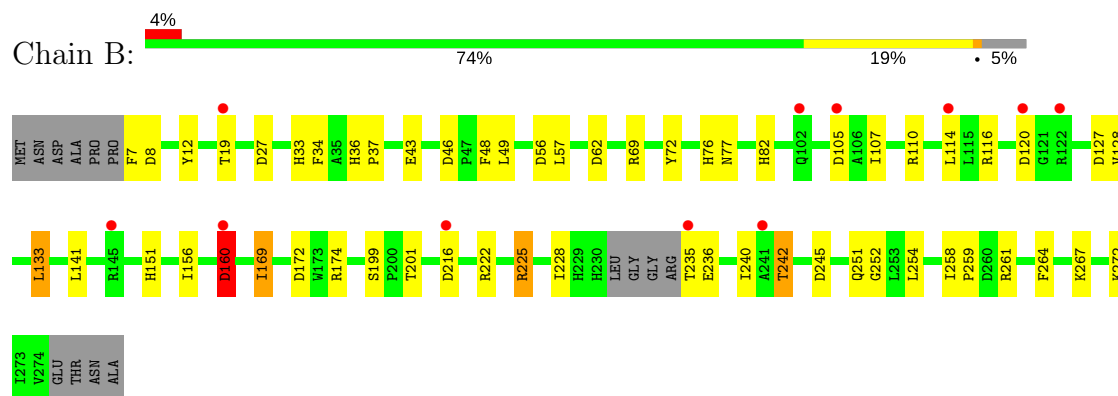
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: ARYLAMINE N-ACETYLTRANSFERASE 1



#### • Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.24Å 97.30Å 114.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.54 – 2.00 25.05 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (74.54-2.00) 98.4 (25.05-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.195 , 0.249 0.199 , 0.243	Depositor DCC
$R_{free}$ test set	2025 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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

### 5.1 Standard geometry

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	0.70	0/2148	0.92	9/2916 (0.3%)
1	B	0.71	0/2123	0.88	8/2882 (0.3%)
All	All	0.70	0/4271	0.90	17/5798 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	122	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	B	110	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	A	216	ASP	CB-CG-OD2	7.93	125.44	118.30
1	B	46	ASP	CB-CG-OD2	7.50	125.05	118.30
1	A	120	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	46	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	160	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	216	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	8	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	120	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	188	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	260	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	56	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	172	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	161	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	56	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	2099	0	2081	28	0
1	B	2075	0	2056	29	0
2	A	139	0	0	8	0
2	B	117	0	0	2	0
All	All	4430	0	4137	57	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.

All (57) 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:134:THR:HB	2:A:2071:HOH:O	1.66	0.93
1:A:8:ASP:H	1:A:61:GLN:HE22	1.13	0.92
1:B:57:LEU:HD13	1:B:82:HIS:CD2	2.08	0.88
1:B:77:ASN:HD21	1:B:128:VAL:H	1.26	0.81
1:B:33:HIS:HE1	1:B:127:ASP:H	1.34	0.74
1:A:36:HIS:HE1	1:A:76:HIS:ND1	1.87	0.73
1:A:12:TYR:OH	1:A:36:HIS:HD2	1.73	0.71
1:A:7:PHE:HD1	1:A:57:LEU:HD11	1.55	0.71
1:A:8:ASP:H	1:A:61:GLN:NE2	1.87	0.70
1:B:33:HIS:CE1	1:B:127:ASP:H	2.10	0.69
1:B:199:SER:OG	1:B:201:THR:HG22	1.93	0.68
1:A:33:HIS:CE1	1:A:127:ASP:H	2.13	0.66
1:A:262:THR:HG23	2:A:2136:HOH:O	1.97	0.63
1:B:12:TYR:OH	1:B:36:HIS:HD2	1.83	0.62
1:B:48:PHE:CZ	1:B:267:LYS:HG2	2.34	0.62
1:B:242:THR:HG22	1:B:245:ASP:H	1.66	0.61
1:B:251:GLN:HE22	1:B:261:ARG:HH11	1.49	0.60
1:A:33:HIS:HE1	1:A:127:ASP:H	1.50	0.60
1:B:36:HIS:HE1	1:B:76:HIS:ND1	2.00	0.59
1:A:49:LEU:HD13	2:A:2021:HOH:O	2.04	0.57
1:B:169:ILE:HG13	1:B:174:ARG:HD2	1.87	0.57
1:B:77:ASN:HD21	1:B:128:VAL:N	2.00	0.56
1:B:49:LEU:HD21	1:B:264:PHE:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:HIS:O	2:A:2122:HOH:O	2.18	0.54
1:B:133:LEU:C	1:B:133:LEU:HD12	2.29	0.54
1:B:7:PHE:HD1	1:B:57:LEU:HD11	1.72	0.54
1:A:122:ARG:HD2	1:A:124:TYR:OH	2.08	0.53
1:B:77:ASN:ND2	1:B:128:VAL:H	2.01	0.53
1:A:57:LEU:HD13	1:A:82:HIS:CD2	2.42	0.53
1:A:134:THR:HG21	2:A:2066:HOH:O	2.09	0.53
1:B:251:GLN:HE22	1:B:261:ARG:NH1	2.07	0.52
1:B:225:ARG:HG2	2:B:2102:HOH:O	2.10	0.51
1:A:7:PHE:CD1	1:A:57:LEU:HD11	2.40	0.51
1:B:69:ARG:HD2	2:B:2111:HOH:O	2.11	0.50
1:A:49:LEU:CD1	2:A:2021:HOH:O	2.60	0.49
1:A:7:PHE:HB2	1:A:57:LEU:HD21	1.94	0.49
1:A:105:ASP:HB3	1:A:107:ILE:O	2.13	0.48
1:A:122:ARG:HG3	1:A:140:LEU:CD1	2.43	0.48
1:A:134:THR:O	1:A:218:ARG:NH1	2.40	0.48
1:A:207:SER:HA	1:A:273:ILE:HD11	1.95	0.48
1:B:34:PHE:HE1	1:B:151:HIS:HE1	1.63	0.47
1:B:36:HIS:HB3	1:B:37:PRO:HD3	1.96	0.47
1:B:141:LEU:HD12	1:B:156:ILE:HD13	1.98	0.45
1:A:36:HIS:HB3	1:A:37:PRO:HD3	1.99	0.44
1:B:240:ILE:HG23	1:B:245:ASP:HB3	2.00	0.43
1:A:228:ILE:O	1:A:235:THR:HA	2.18	0.42
1:B:7:PHE:CD1	1:B:57:LEU:HD11	2.53	0.42
1:A:122:ARG:NH2	2:A:2060:HOH:O	2.53	0.42
1:A:216:ASP:OD1	1:A:217:ARG:NH2	2.51	0.42
1:B:225:ARG:HG2	1:B:225:ARG:O	2.17	0.42
1:B:228:ILE:O	1:B:235:THR:HA	2.21	0.41
1:A:54:ARG:HG3	2:A:2027:HOH:O	2.20	0.41
1:B:258:ILE:HA	1:B:259:PRO:HD3	1.92	0.41
1:A:272:LYS:HB3	1:A:275:GLU:HB2	2.03	0.40
1:B:105:ASP:HB3	1:B:107:ILE:O	2.21	0.40
1:A:216:ASP:N	1:A:216:ASP:OD2	2.52	0.40
1:B:160:ASP:OD2	1:B:160:ASP:N	2.53	0.40

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	263/278 (95%)	252 (96%)	11 (4%)	0	100	100
1	B	260/278 (94%)	250 (96%)	9 (4%)	1 (0%)	38	33
All	All	523/556 (94%)	502 (96%)	20 (4%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	GLY

### 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	216/223 (97%)	205 (95%)	11 (5%)	28	22
1	B	213/223 (96%)	197 (92%)	16 (8%)	16	10
All	All	429/446 (96%)	402 (94%)	27 (6%)	21	15

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	72	TYR
1	A	91	VAL
1	A	102	GLN
1	A	114	LEU

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Mol	Chain	Res	Type
1	A	119	LEU
1	A	160	ASP
1	A	190	SER
1	A	216	ASP
1	A	272	LYS
1	A	274	VAL
1	B	19	THR
1	B	27	ASP
1	B	43	GLU
1	B	62	ASP
1	B	72	TYR
1	B	114	LEU
1	B	116	ARG
1	B	133	LEU
1	B	160	ASP
1	B	169	ILE
1	B	222	ARG
1	B	225	ARG
1	B	236	GLU
1	B	242	THR
1	B	254	LEU
1	B	272	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	36	HIS
1	A	61	GLN
1	A	237	GLN
1	B	33	HIS
1	B	36	HIS
1	B	77	ASN
1	B	251	GLN

### 5.3.3 RNA ⓘ

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

### 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	267/278 (96%)	0.18	15 (5%) 25 25	13, 26, 47, 58	0
1	B	264/278 (94%)	0.18	11 (4%) 37 37	13, 27, 44, 54	0
All	All	531/556 (95%)	0.18	26 (4%) 30 30	13, 27, 46, 58	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	ASP	4.5
1	B	160	ASP	3.9
1	A	231	LEU	3.9
1	B	19	THR	3.8
1	A	104	GLU	3.8
1	B	235	THR	3.7
1	A	105	ASP	3.6
1	A	106	ALA	3.5
1	A	160	ASP	3.4
1	B	145	ARG	2.8
1	A	275	GLU	2.7
1	A	66	LEU	2.7
1	B	120	ASP	2.7
1	A	6	PRO	2.6
1	A	19	THR	2.5
1	A	262	THR	2.4
1	B	102	GLN	2.4
1	B	105	ASP	2.4
1	B	122	ARG	2.4
1	B	241	ALA	2.4
1	B	114	LEU	2.2
1	A	270	GLU	2.1
1	A	200	PRO	2.1
1	A	224	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	216	ASP	2.0
1	A	102	GLN	2.0

## 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 [i](#)

There are no such residues in this entry.