



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:07 PM GMT

PDB ID : 4NV8
Title : Crystal Structure of Mesorhizobium Loti Arylamine N-acetyltransferase F42W Mutant
Authors : Xu, X.M.; Haouz, A.; Weber, P.; Li de la sierra-gallay, I.; Kubiak, X.; Dupret, J.-M.; Rodrigues-lima, F.
Deposited on : 2013-12-05
Resolution : 1.84 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
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

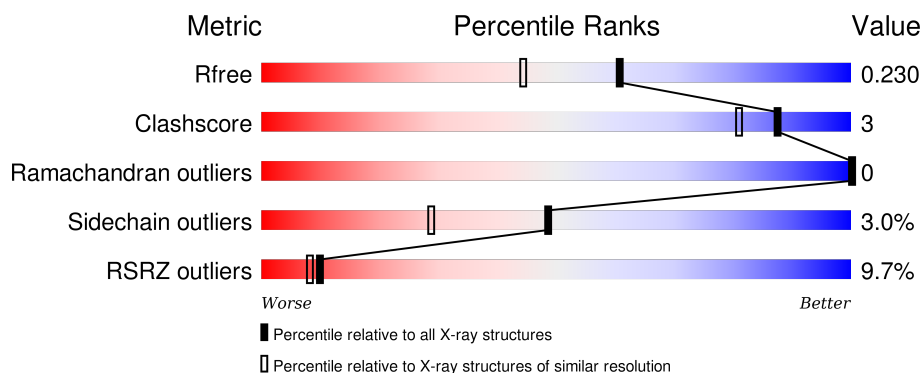
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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	312	<div> <div>12%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>
1	B	312	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4449 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
1	A	270	Total	C	N	O	S	0	1	0
			2128	1359	382	384	3			
1	B	268	Total	C	N	O	S	0	0	0
			2104	1345	376	380	3			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	INITIATING METHIONINE	UNP Q98D42
A	-32	GLY	-	EXPRESSION TAG	UNP Q98D42
A	-31	SER	-	EXPRESSION TAG	UNP Q98D42
A	-30	SER	-	EXPRESSION TAG	UNP Q98D42
A	-29	HIS	-	EXPRESSION TAG	UNP Q98D42
A	-28	HIS	-	EXPRESSION TAG	UNP Q98D42
A	-27	HIS	-	EXPRESSION TAG	UNP Q98D42
A	-26	HIS	-	EXPRESSION TAG	UNP Q98D42
A	-25	HIS	-	EXPRESSION TAG	UNP Q98D42
A	-24	HIS	-	EXPRESSION TAG	UNP Q98D42
A	-23	SER	-	EXPRESSION TAG	UNP Q98D42
A	-22	SER	-	EXPRESSION TAG	UNP Q98D42
A	-21	GLY	-	EXPRESSION TAG	UNP Q98D42
A	-20	LEU	-	EXPRESSION TAG	UNP Q98D42
A	-19	VAL	-	EXPRESSION TAG	UNP Q98D42
A	-18	PRO	-	EXPRESSION TAG	UNP Q98D42
A	-17	ARG	-	EXPRESSION TAG	UNP Q98D42
A	-16	GLY	-	EXPRESSION TAG	UNP Q98D42
A	-15	SER	-	EXPRESSION TAG	UNP Q98D42
A	-14	HIS	-	EXPRESSION TAG	UNP Q98D42
A	-13	MET	-	EXPRESSION TAG	UNP Q98D42
A	-12	ALA	-	EXPRESSION TAG	UNP Q98D42
A	-11	SER	-	EXPRESSION TAG	UNP Q98D42
A	-10	ASN	-	EXPRESSION TAG	UNP Q98D42
A	-9	THR	-	EXPRESSION TAG	UNP Q98D42

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	EXPRESSION TAG	UNP Q98D42
A	-7	GLY	-	EXPRESSION TAG	UNP Q98D42
A	-6	GLN	-	EXPRESSION TAG	UNP Q98D42
A	-5	GLN	-	EXPRESSION TAG	UNP Q98D42
A	-4	MET	-	EXPRESSION TAG	UNP Q98D42
A	-3	GLY	-	EXPRESSION TAG	UNP Q98D42
A	-2	ARG	-	EXPRESSION TAG	UNP Q98D42
A	-1	GLY	-	EXPRESSION TAG	UNP Q98D42
A	0	SER	-	EXPRESSION TAG	UNP Q98D42
A	42	TRP	PHE	ENGINEERED MUTATION	UNP Q98D42
B	-33	MET	-	INITIATING METHIONINE	UNP Q98D42
B	-32	GLY	-	EXPRESSION TAG	UNP Q98D42
B	-31	SER	-	EXPRESSION TAG	UNP Q98D42
B	-30	SER	-	EXPRESSION TAG	UNP Q98D42
B	-29	HIS	-	EXPRESSION TAG	UNP Q98D42
B	-28	HIS	-	EXPRESSION TAG	UNP Q98D42
B	-27	HIS	-	EXPRESSION TAG	UNP Q98D42
B	-26	HIS	-	EXPRESSION TAG	UNP Q98D42
B	-25	HIS	-	EXPRESSION TAG	UNP Q98D42
B	-24	HIS	-	EXPRESSION TAG	UNP Q98D42
B	-23	SER	-	EXPRESSION TAG	UNP Q98D42
B	-22	SER	-	EXPRESSION TAG	UNP Q98D42
B	-21	GLY	-	EXPRESSION TAG	UNP Q98D42
B	-20	LEU	-	EXPRESSION TAG	UNP Q98D42
B	-19	VAL	-	EXPRESSION TAG	UNP Q98D42
B	-18	PRO	-	EXPRESSION TAG	UNP Q98D42
B	-17	ARG	-	EXPRESSION TAG	UNP Q98D42
B	-16	GLY	-	EXPRESSION TAG	UNP Q98D42
B	-15	SER	-	EXPRESSION TAG	UNP Q98D42
B	-14	HIS	-	EXPRESSION TAG	UNP Q98D42
B	-13	MET	-	EXPRESSION TAG	UNP Q98D42
B	-12	ALA	-	EXPRESSION TAG	UNP Q98D42
B	-11	SER	-	EXPRESSION TAG	UNP Q98D42
B	-10	ASN	-	EXPRESSION TAG	UNP Q98D42
B	-9	THR	-	EXPRESSION TAG	UNP Q98D42
B	-8	GLY	-	EXPRESSION TAG	UNP Q98D42
B	-7	GLY	-	EXPRESSION TAG	UNP Q98D42
B	-6	GLN	-	EXPRESSION TAG	UNP Q98D42
B	-5	GLN	-	EXPRESSION TAG	UNP Q98D42
B	-4	MET	-	EXPRESSION TAG	UNP Q98D42
B	-3	GLY	-	EXPRESSION TAG	UNP Q98D42
B	-2	ARG	-	EXPRESSION TAG	UNP Q98D42

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP Q98D42
B	0	SER	-	EXPRESSION TAG	UNP Q98D42
B	42	TRP	PHE	ENGINEERED MUTATION	UNP Q98D42

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	99	Total O 99 99	0	0
2	B	118	Total O 118 118	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	52.86Å 115.08Å 115.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.01 – 1.84 32.01 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.01-1.84) 99.6 (32.01-1.84)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.204 , 0.228 0.208 , 0.230	Depositor DCC
R_{free} test set	3126 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.3	EDS
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 61770 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4449	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.57	0/2182	0.74	1/2962 (0.0%)
1	B	0.68	1/2155 (0.0%)	0.77	0/2927
All	All	0.63	1/4337 (0.0%)	0.75	1/5889 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	TYR	CE1-CZ	-5.24	1.31	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH2	-5.61	117.49	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	2128	0	2117	13	0
1	B	2104	0	2089	10	0
2	A	99	0	0	1	0
2	B	118	0	0	0	0
All	All	4449	0	4206	22	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 3.

All (22) 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:51:ARG:HH12	1:B:259:PRO:HG2	1.56	0.69
1:A:51:ARG:HH12	1:A:259:PRO:HG2	1.58	0.69
1:B:46:ASP:OD1	1:B:51:ARG:NH1	2.26	0.69
1:B:51:ARG:NH1	1:B:259:PRO:HG2	2.09	0.68
1:A:46:ASP:OD1	1:A:51:ARG:NH1	2.28	0.67
1:A:51:ARG:NH1	1:A:259:PRO:HG2	2.13	0.63
1:A:134:THR:HG21	2:A:382:HOH:O	2.06	0.56
1:A:7:PHE:HD1	1:A:57:LEU:HD11	1.72	0.55
1:A:219:TYR:HB3	1:A:254:LEU:HD21	1.89	0.54
1:A:194:TYR:CE2	1:B:194:TYR:CE2	2.98	0.52
1:B:37:PRO:HB3	1:B:134:THR:HG21	1.94	0.49
1:B:267:LYS:HA	1:B:270:GLU:HG2	1.94	0.48
1:A:230:HIS:HE1	1:A:236:GLU:OE2	1.97	0.47
1:B:85:LYS:HG3	1:B:91:VAL:CG1	2.45	0.47
1:B:7:PHE:HD1	1:B:57:LEU:HD11	1.80	0.46
1:B:69:ARG:HG2	1:B:257:ILE:HB	1.98	0.46
1:A:85:LYS:HG3	1:A:91:VAL:CG1	2.47	0.44
1:A:251:GLN:HG2	1:A:256:ILE:O	2.18	0.44
1:A:230:HIS:CE1	1:A:236:GLU:OE2	2.71	0.43
1:A:103:SER:O	1:A:106:ALA:N	2.52	0.43
1:A:212:ARG:NE	1:A:254:LEU:O	2.45	0.42
1:B:100:TRP:HH2	1:B:169:ILE:CD1	2.35	0.40

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	Percentiles	
1	A	267/312 (86%)	258 (97%)	9 (3%)	0	100	100
1	B	264/312 (85%)	255 (97%)	9 (3%)	0	100	100
All	All	531/624 (85%)	513 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	218/249 (88%)	213 (98%)	5 (2%)	58	41
1	B	215/249 (86%)	207 (96%)	8 (4%)	41	20
All	All	433/498 (87%)	420 (97%)	13 (3%)	48	29

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	72	TYR
1	A	114	LEU
1	A	134	THR
1	A	234	ARG
1	B	43	GLU
1	B	66	LEU
1	B	72	TYR
1	B	105	ASP
1	B	114	LEU
1	B	158	GLU
1	B	207	SER
1	B	234	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	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 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, 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	270/312 (86%)	0.60	37 (13%) 4 3	19, 33, 60, 80	0
1	B	268/312 (85%)	0.19	15 (5%) 28 25	17, 28, 54, 76	0
All	All	538/624 (86%)	0.40	52 (9%) 10 8	17, 30, 58, 80	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	GLY	7.2
1	A	5	PRO	6.9
1	A	106	ALA	6.1
1	B	159	ALA	5.3
1	A	231	LEU	4.7
1	B	161	ASP	4.2
1	B	160	ASP	4.2
1	A	201	THR	4.1
1	B	231	LEU	4.0
1	A	234	ARG	4.0
1	A	103	SER	3.9
1	A	216	ASP	3.8
1	B	105	ASP	3.7
1	A	161	ASP	3.7
1	B	234	ARG	3.6
1	A	128	VAL	3.6
1	A	274	VAL	3.4
1	A	160	ASP	3.4
1	A	104	GLU	3.3
1	A	135	LEU	3.2
1	B	232	GLY	3.1
1	A	233	GLY	3.0
1	B	144	GLY	3.0
1	B	5	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	6	PRO	2.9
1	A	114	LEU	2.8
1	B	275	GLU	2.8
1	B	274	VAL	2.7
1	A	237	GLN	2.7
1	A	240	ILE	2.7
1	A	241	ALA	2.6
1	A	230	HIS	2.6
1	A	40	ILE	2.6
1	A	275	GLU	2.6
1	B	106	ALA	2.6
1	A	125	ILE	2.5
1	A	205	LEU	2.5
1	B	225	ARG	2.5
1	A	236	GLU	2.4
1	A	217	ARG	2.4
1	A	159	ALA	2.3
1	A	238	THR	2.3
1	A	239	GLU	2.3
1	A	101	GLY	2.3
1	A	242	THR	2.3
1	B	6	PRO	2.2
1	A	115	LEU	2.2
1	A	102	GLN	2.2
1	A	269	ARG	2.2
1	B	230	HIS	2.1
1	A	235	THR	2.1
1	A	203	HIS	2.1

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.