



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:16 pm GMT

PDB ID : 2NTN  
Title : Crystal structure of MabA-C60V/G139A/S144L  
Authors : Poncet-Montange, G.; Ducasse-Cabanot, S.; Quemard, A.; Labesse, G.;  
Cohen-Gonsaud, M.  
Deposited on : 2006-11-08  
Resolution : 2.30 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

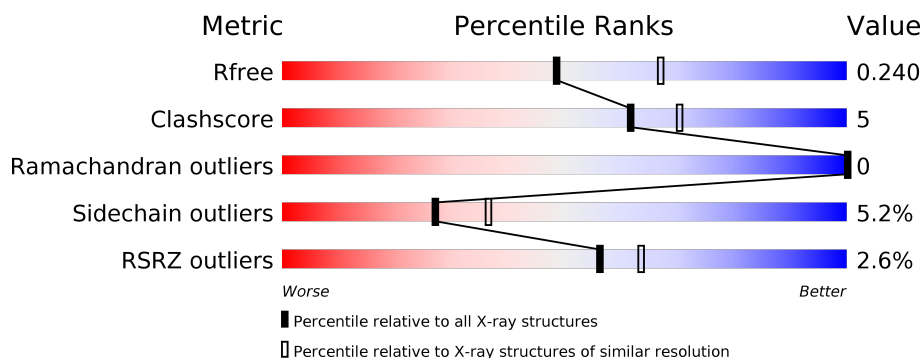
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	267	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	267	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>10%</div> <div>•</div> <div>22%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3304 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 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1564	976	284	298	6			
1	B	207	Total	C	N	O	S	0	0	0
			1501	937	274	284	6			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P0A5Y4
A	-18	GLY	-	EXPRESSION TAG	UNP P0A5Y4
A	-17	SER	-	EXPRESSION TAG	UNP P0A5Y4
A	-16	SER	-	EXPRESSION TAG	UNP P0A5Y4
A	-15	HIS	-	EXPRESSION TAG	UNP P0A5Y4
A	-14	HIS	-	EXPRESSION TAG	UNP P0A5Y4
A	-13	HIS	-	EXPRESSION TAG	UNP P0A5Y4
A	-12	HIS	-	EXPRESSION TAG	UNP P0A5Y4
A	-11	HIS	-	EXPRESSION TAG	UNP P0A5Y4
A	-10	HIS	-	EXPRESSION TAG	UNP P0A5Y4
A	-9	SER	-	EXPRESSION TAG	UNP P0A5Y4
A	-8	SER	-	EXPRESSION TAG	UNP P0A5Y4
A	-7	GLY	-	EXPRESSION TAG	UNP P0A5Y4
A	-6	LEU	-	EXPRESSION TAG	UNP P0A5Y4
A	-5	VAL	-	EXPRESSION TAG	UNP P0A5Y4
A	-4	PRO	-	EXPRESSION TAG	UNP P0A5Y4
A	-3	ARG	-	EXPRESSION TAG	UNP P0A5Y4
A	-2	GLY	-	EXPRESSION TAG	UNP P0A5Y4
A	-1	SER	-	EXPRESSION TAG	UNP P0A5Y4
A	0	HIS	-	EXPRESSION TAG	UNP P0A5Y4
A	60	VAL	CYS	ENGINEERED	UNP P0A5Y4
A	139	ALA	GLY	ENGINEERED	UNP P0A5Y4
A	144	LEU	SER	ENGINEERED	UNP P0A5Y4
B	-19	MET	-	EXPRESSION TAG	UNP P0A5Y4
B	-18	GLY	-	EXPRESSION TAG	UNP P0A5Y4

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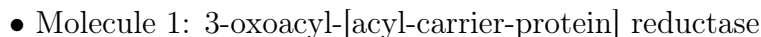
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	EXPRESSION TAG	UNP P0A5Y4
B	-16	SER	-	EXPRESSION TAG	UNP P0A5Y4
B	-15	HIS	-	EXPRESSION TAG	UNP P0A5Y4
B	-14	HIS	-	EXPRESSION TAG	UNP P0A5Y4
B	-13	HIS	-	EXPRESSION TAG	UNP P0A5Y4
B	-12	HIS	-	EXPRESSION TAG	UNP P0A5Y4
B	-11	HIS	-	EXPRESSION TAG	UNP P0A5Y4
B	-10	HIS	-	EXPRESSION TAG	UNP P0A5Y4
B	-9	SER	-	EXPRESSION TAG	UNP P0A5Y4
B	-8	SER	-	EXPRESSION TAG	UNP P0A5Y4
B	-7	GLY	-	EXPRESSION TAG	UNP P0A5Y4
B	-6	LEU	-	EXPRESSION TAG	UNP P0A5Y4
B	-5	VAL	-	EXPRESSION TAG	UNP P0A5Y4
B	-4	PRO	-	EXPRESSION TAG	UNP P0A5Y4
B	-3	ARG	-	EXPRESSION TAG	UNP P0A5Y4
B	-2	GLY	-	EXPRESSION TAG	UNP P0A5Y4
B	-1	SER	-	EXPRESSION TAG	UNP P0A5Y4
B	0	HIS	-	EXPRESSION TAG	UNP P0A5Y4
B	60	VAL	CYS	ENGINEERED	UNP P0A5Y4
B	139	ALA	GLY	ENGINEERED	UNP P0A5Y4
B	144	LEU	SER	ENGINEERED	UNP P0A5Y4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	114	Total	O	0	0
			114	114		



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.61Å 117.28Å 52.27Å 90.00° 121.90° 90.00°	Depositor
Resolution (Å)	24.00 – 2.30 23.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (24.00-2.30) 92.5 (23.70-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.177 , 0.238 0.178 , 0.240	Depositor DCC
$R_{free}$ test set	868 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% 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	0.49	0/1583	0.71	5/2139 (0.2%)
1	B	0.49	0/1519	0.70	5/2050 (0.2%)
All	All	0.49	0/3102	0.70	10/4189 (0.2%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	61	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	228	ASP	CB-CG-OD2	6.16	123.85	118.30
1	B	66	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	187	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	69	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	66	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	228	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	187	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	69	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ALA	Peptide

## 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	1564	0	1556	19	0
1	B	1501	0	1516	12	0
2	A	125	0	0	3	0
2	B	114	0	0	0	0
All	All	3304	0	3072	31	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 5.

All (31) 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:90:GLY:O	1:B:91:LEU:HG	1.55	1.05
1:B:51:ALA:HB2	1:B:57:GLY:HA3	1.83	0.61
1:B:139:ALA:HB1	1:B:157:LYS:HG3	1.83	0.60
1:A:18:VAL:HG22	1:A:84:VAL:HB	1.86	0.57
1:A:152:ASN:HD22	1:A:152:ASN:N	2.03	0.55
1:A:60:VAL:HG22	1:A:71:ALA:HB2	1.89	0.55
1:A:156:SER:O	1:A:160:VAL:HG23	2.08	0.54
1:B:76:GLU:HG2	1:B:81:PRO:HA	1.90	0.53
1:A:128:GLN:O	1:A:131:LYS:NZ	2.37	0.53
1:A:33:GLN:OE1	2:A:365:HOH:O	2.19	0.53
1:B:185:TYR:HD1	1:B:206:ILE:HD11	1.73	0.53
1:A:90:GLY:HA3	1:A:112:ASN:OD1	2.10	0.52
1:A:139:ALA:HB1	1:A:157:LYS:CG	2.40	0.51
1:A:139:ALA:HB1	1:A:157:LYS:HG2	1.93	0.50
1:B:31:ILE:HG21	1:B:86:VAL:HG11	1.97	0.47
1:B:100:MET:CE	1:B:104:LYS:HB2	2.45	0.47
1:A:171:LEU:HB3	1:A:176:VAL:HB	1.98	0.46
1:B:185:TYR:CD1	1:B:206:ILE:HD11	2.51	0.46
1:A:100:MET:CE	1:A:104:LYS:HB2	2.45	0.46
1:A:152:ASN:ND2	1:A:152:ASN:N	2.64	0.46
1:B:117:PHE:O	1:B:121:GLN:HB2	2.17	0.45
1:A:152:ASN:H	1:A:152:ASN:ND2	2.15	0.45
1:A:76:GLU:HG3	2:A:358:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:O	1:A:118:ARG:HD2	2.16	0.44
1:A:45:THR:HA	1:A:58:VAL:O	2.20	0.42
1:A:100:MET:N	2:A:348:HOH:O	2.53	0.42
1:B:24:ASN:ND2	1:B:49:SER:OG	2.53	0.41
1:A:10:LYS:HA	1:A:11:PRO:HD3	1.98	0.41
1:A:21:THR:O	1:A:88:ASN:HB2	2.21	0.41
1:B:62:VAL:O	1:B:118:ARG:HD2	2.20	0.41
1:B:21:THR:O	1:B:88:ASN:HB2	2.21	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	210/267 (79%)	201 (96%)	9 (4%)	0	100	100
1	B	199/267 (74%)	193 (97%)	6 (3%)	0	100	100
All	All	409/534 (77%)	394 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	155/199 (78%)	146 (94%)	9 (6%)	23	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	152/199 (76%)	145 (95%)	7 (5%)	31	42
All	All	307/398 (77%)	291 (95%)	16 (5%)	27	36

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	63	THR
1	A	91	LEU
1	A	121	GLN
1	A	141	VAL
1	A	150	GLN
1	A	152	ASN
1	A	157	LYS
1	A	200	GLN
1	B	19	LEU
1	B	47	ARG
1	B	84	VAL
1	B	91	LEU
1	B	121	GLN
1	B	157	LYS
1	B	188	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	B	112	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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, 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	218/267 (81%)	-0.08	9 (4%) 38 45	18, 23, 34, 49	2 (0%)
1	B	207/267 (77%)	-0.19	2 (0%) 82 86	18, 23, 30, 36	6 (2%)
All	All	425/534 (79%)	-0.13	11 (2%) 56 63	18, 23, 32, 49	8 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ALA	9.2
1	A	194	LEU	4.8
1	A	189	ASP	4.7
1	A	190	MET	3.5
1	A	188	THR	2.5
1	A	191	THR	2.5
1	A	192	ARG	2.5
1	B	245	MET	2.5
1	B	205	PHE	2.4
1	A	195	ASP	2.1
1	A	199	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.