



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 05:30 PM GMT

PDB ID : 3MJI
Title : Activation of catalytic cysteine without a base in a Mutant Penicillin Acylase Precursor
Authors : Pathak, M.C.; Suresh, C.G.; Dodson, G.G; Murshudov, G.N.
Deposited on : 2010-04-12
Resolution : 2.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

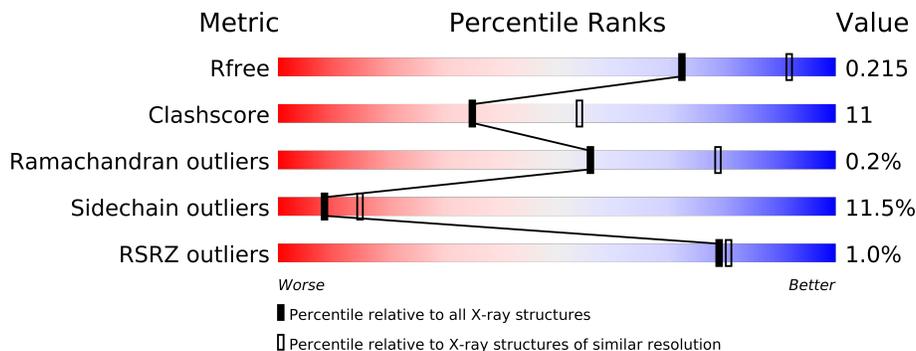
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. 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	338	
1	B	338	
1	C	338	
1	D	338	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10729 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 Penicillin acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2606	1659	427	507	13	0	0	0
1	B	334	2606	1659	427	507	13	0	0	0
1	C	333	2599	1654	426	506	13	0	0	0
1	D	333	2599	1654	426	506	13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

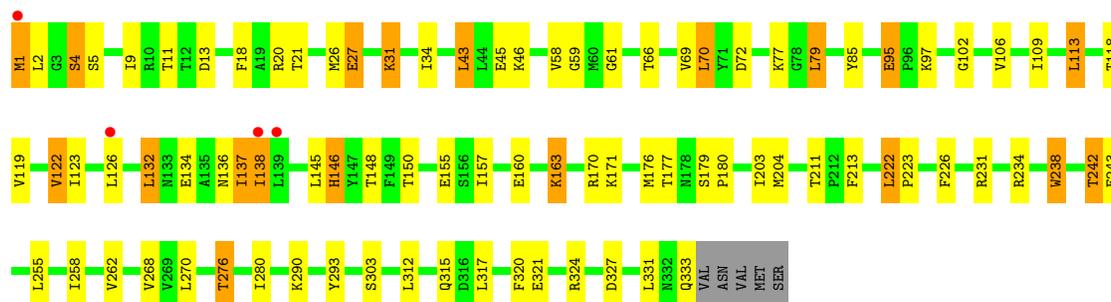
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	CYS	CONFLICT	UNP P12256
A	101	ARG	THR	CONFLICT	UNP P12256
B	4	SER	CYS	CONFLICT	UNP P12256
B	101	ARG	THR	CONFLICT	UNP P12256
C	4	SER	CYS	CONFLICT	UNP P12256
C	101	ARG	THR	CONFLICT	UNP P12256
D	4	SER	CYS	CONFLICT	UNP P12256
D	101	ARG	THR	CONFLICT	UNP P12256

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total 90	O 90	0	0
2	B	69	Total 69	O 69	0	0
2	C	73	Total 73	O 73	0	0
2	D	87	Total 87	O 87	0	0

- Molecule 1: Penicillin acylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.64Å 90.09Å 102.27Å 90.00° 102.13° 90.00°	Depositor
Resolution (Å)	19.95 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.95-2.50) 99.0 (19.95-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.50Å)	Xtrriage
Refinement program	REFMAC 5.6.0041	Depositor
R, R_{free}	0.166 , 0.211 0.172 , 0.215	Depositor DCC
R_{free} test set	3170 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	26.7	Xtrriage
Anisotropy	0.473	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 14.6	EDS
Estimated twinning fraction	0.901 for H, K, L 0.099 for L, -K, H 0.124 for l,-k,h	Xtrriage
Reported twinning fraction	0.901 for H, K, L 0.099 for L, -K, H	Depositor
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Outliers	2 of 62981 reflections (0.003%)	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10729	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2485e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities 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	1.23	3/2661 (0.1%)	0.99	2/3616 (0.1%)
1	B	1.15	3/2661 (0.1%)	0.99	4/3616 (0.1%)
1	C	1.15	2/2654 (0.1%)	0.98	3/3606 (0.1%)
1	D	1.12	2/2654 (0.1%)	1.00	2/3606 (0.1%)
All	All	1.16	10/10630 (0.1%)	0.99	11/14444 (0.1%)

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	C	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	SER	CB-OG	-5.93	1.34	1.42
1	B	209	ASP	CB-CG	-5.92	1.39	1.51
1	D	226	PHE	CE1-CZ	5.62	1.48	1.37
1	C	179	SER	CB-OG	-5.49	1.35	1.42
1	A	160	GLU	CG-CD	5.44	1.60	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	LEU	CA-CB-CG	5.92	128.92	115.30
1	D	70	LEU	CA-CB-CG	-5.78	102.01	115.30
1	B	233	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	190	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	C	126	LEU	CB-CG-CD1	5.33	120.07	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	136	ASN	Peptide
1	C	139	LEU	Peptide

5.2 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 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	2606	0	2587	48	0
1	B	2606	0	2587	57	0
1	C	2599	0	2578	58	0
1	D	2599	0	2578	67	0
2	A	90	0	0	2	0
2	B	69	0	0	1	0
2	C	73	0	0	0	0
2	D	87	0	0	3	0
All	All	10729	0	10330	221	0

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 11.

The worst 5 of 221 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:137:ILE:O	1:C:140:GLY:HA2	1.34	1.27
1:A:24:PHE:HB3	1:A:280:ILE:CD1	1.66	1.26
1:C:137:ILE:HD12	1:C:137:ILE:H	1.07	1.13
1:C:137:ILE:H	1:C:137:ILE:CD1	1.63	1.11
1:C:136:ASN:HB3	1:C:137:ILE:C	1.73	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

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	332/338 (98%)	316 (95%)	15 (4%)	1 (0%)	50	73
1	B	332/338 (98%)	309 (93%)	22 (7%)	1 (0%)	50	73
1	C	331/338 (98%)	311 (94%)	20 (6%)	0	100	100
1	D	331/338 (98%)	313 (95%)	17 (5%)	1 (0%)	50	73
All	All	1326/1352 (98%)	1249 (94%)	74 (6%)	3 (0%)	56	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS
1	A	119	VAL
1	B	180	PRO

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	290/294 (99%)	268 (92%)	22 (8%)	19	33
1	B	290/294 (99%)	250 (86%)	40 (14%)	5	9
1	C	289/294 (98%)	253 (88%)	36 (12%)	7	12
1	D	289/294 (98%)	254 (88%)	35 (12%)	7	13
All	All	1158/1176 (98%)	1025 (88%)	133 (12%)	8	15

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	331	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	85	TYR
1	D	242	THR
1	B	333	GLN
1	C	29	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	315	GLN
1	B	188	ASN

5.3.3 RNA [i](#)

There are no RNA chains 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

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	334/338 (98%)	-0.24	3 (0%) 81 82	15, 24, 42, 71	0
1	B	334/338 (98%)	-0.19	6 (1%) 65 68	16, 26, 48, 67	0
1	C	333/338 (98%)	-0.25	1 (0%) 91 93	15, 26, 44, 66	0
1	D	333/338 (98%)	-0.22	4 (1%) 75 77	15, 26, 49, 62	0
All	All	1334/1352 (98%)	-0.22	14 (1%) 79 81	15, 25, 46, 71	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	ILE	6.0
1	B	138	ILE	4.3
1	A	26	MET	3.2
1	D	1	MET	3.0
1	A	2	LEU	2.9

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.