wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 02:41 PM EDT

PDB ID	:	2AJ9
Title	:	X-ray crystal structure of W42A,R161A double mutant of Mycobacterium tuberculosis beta-ketoacyl-ACP synthase III
Authors	:	Brown, A.K.; Sridharan, S.; Kremer, L.; Lindenberg, S.; Dover, L.G.; Sacchettini, J.C.; Besra, G.S.
Deposited on	:	2005-08-01
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

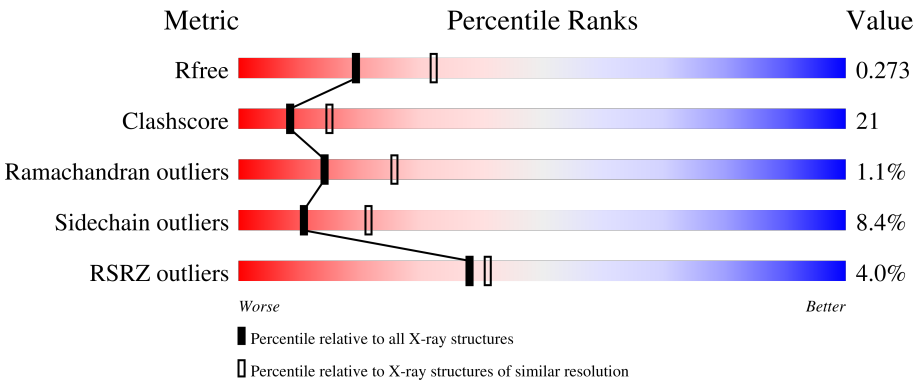
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	356	3% 58% 32% • • 6%
1	B	356	5% 55% 33% • • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4955 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] synthase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2427	1513	428	472	14	0	0	0
1	B	334	2427	1513	428	472	14	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	cloning artifact	UNP P0A574
A	-19	GLY	-	cloning artifact	UNP P0A574
A	-18	SER	-	cloning artifact	UNP P0A574
A	-17	SER	-	cloning artifact	UNP P0A574
A	-16	HIS	-	expression tag	UNP P0A574
A	-15	HIS	-	expression tag	UNP P0A574
A	-14	HIS	-	expression tag	UNP P0A574
A	-13	HIS	-	expression tag	UNP P0A574
A	-12	HIS	-	expression tag	UNP P0A574
A	-11	HIS	-	expression tag	UNP P0A574
A	-10	SER	-	cloning artifact	UNP P0A574
A	-9	SER	-	cloning artifact	UNP P0A574
A	-8	GLY	-	cloning artifact	UNP P0A574
A	-7	LEU	-	cloning artifact	UNP P0A574
A	-6	VAL	-	cloning artifact	UNP P0A574
A	-5	PRO	-	cloning artifact	UNP P0A574
A	-4	ARG	-	cloning artifact	UNP P0A574
A	-3	GLY	-	cloning artifact	UNP P0A574
A	-2	SER	-	cloning artifact	UNP P0A574
A	-1	VAL	-	cloning artifact	UNP P0A574
A	0	CYS	-	cloning artifact	UNP P0A574
A	42	ALA	TRP	engineered mutation	UNP P0A574
A	161	ALA	ARG	engineered mutation	UNP P0A574
B	-20	MET	-	cloning artifact	UNP P0A574
B	-19	GLY	-	cloning artifact	UNP P0A574

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	cloning artifact	UNP P0A574
B	-17	SER	-	cloning artifact	UNP P0A574
B	-16	HIS	-	expression tag	UNP P0A574
B	-15	HIS	-	expression tag	UNP P0A574
B	-14	HIS	-	expression tag	UNP P0A574
B	-13	HIS	-	expression tag	UNP P0A574
B	-12	HIS	-	expression tag	UNP P0A574
B	-11	HIS	-	expression tag	UNP P0A574
B	-10	SER	-	cloning artifact	UNP P0A574
B	-9	SER	-	cloning artifact	UNP P0A574
B	-8	GLY	-	cloning artifact	UNP P0A574
B	-7	LEU	-	cloning artifact	UNP P0A574
B	-6	VAL	-	cloning artifact	UNP P0A574
B	-5	PRO	-	cloning artifact	UNP P0A574
B	-4	ARG	-	cloning artifact	UNP P0A574
B	-3	GLY	-	cloning artifact	UNP P0A574
B	-2	SER	-	cloning artifact	UNP P0A574
B	-1	VAL	-	cloning artifact	UNP P0A574
B	0	CYS	-	cloning artifact	UNP P0A574
B	42	ALA	TRP	engineered mutation	UNP P0A574
B	161	ALA	ARG	engineered mutation	UNP P0A574

- Molecule 2 is water.

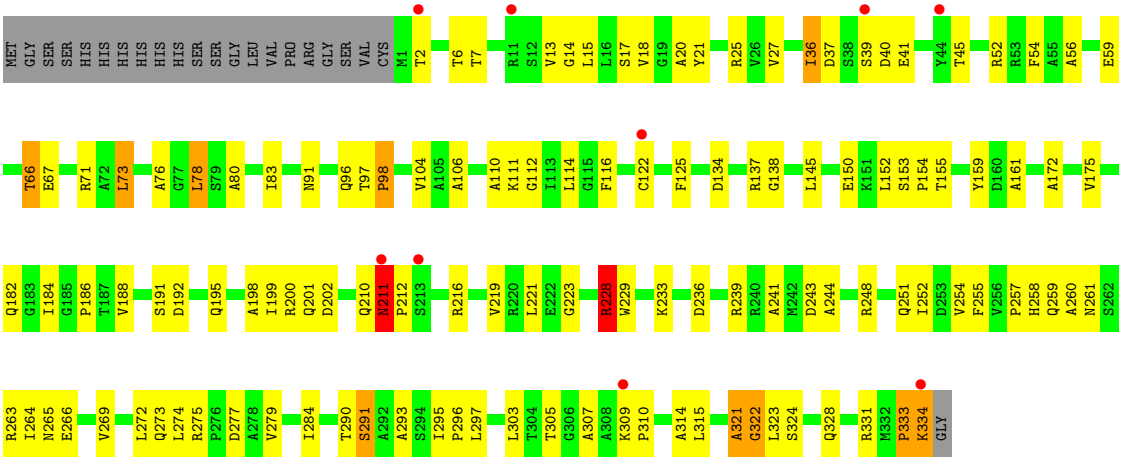
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	62	62	62	0	0
			Total	O		
2	B	39	39	39	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

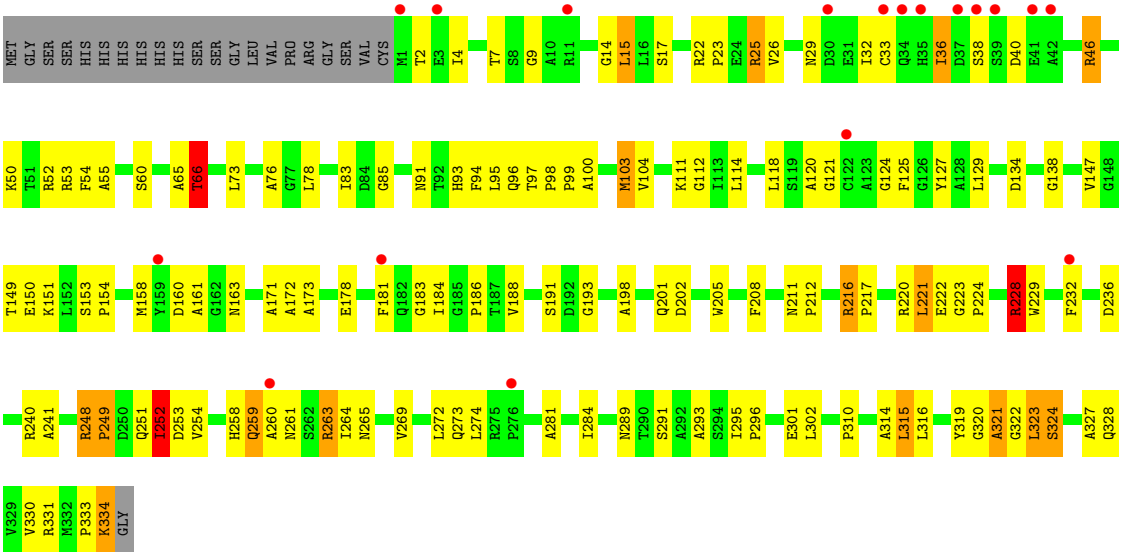
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase III

Chain A:



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase III

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.17Å 56.02Å 88.19Å 90.00° 90.57° 90.00°	Depositor
Resolution (Å)	28.01 – 2.50 28.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (28.01-2.50) 92.2 (28.01-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.279 0.232 , 0.273	Depositor DCC
R_{free} test set	1980 reflections (9.39%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4955	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	2.05	2/2469 (0.1%)	1.05	17/3358 (0.5%)
1	B	0.63	2/2469 (0.1%)	1.09	21/3358 (0.6%)
All	All	1.52	4/4938 (0.1%)	1.07	38/6716 (0.6%)

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	4
1	B	0	8
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	LYS	C-O	97.49	3.08	1.23
1	B	324	SER	C-O	6.79	1.36	1.23
1	B	253	ASP	C-N	5.81	1.47	1.34
1	A	211	ASN	C-N	5.21	1.44	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	228	ARG	NE-CZ-NH1	-12.83	113.89	120.30
1	B	228	ARG	NE-CZ-NH2	11.68	126.14	120.30
1	B	248	ARG	C-N-CD	10.09	149.58	128.40
1	A	211	ASN	C-N-CD	9.77	148.91	128.40
1	A	334	LYS	CA-C-O	9.56	140.18	120.10

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	GLN	Peptide,Mainchain
1	A	211	ASN	Mainchain
1	A	305	THR	Mainchain
1	B	36	ILE	Mainchain
1	B	9	GLY	Mainchain

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	2427	0	2402	106	0
1	B	2427	0	2402	122	0
2	A	62	0	0	3	0
2	B	39	0	0	2	0
All	All	4955	0	4804	201	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 21.

The worst 5 of 201 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:261:ASN:HD22	1:B:264:ILE:HG13	1.26	0.99
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.29	0.95
1:B:258:HIS:CD2	1:B:260:ALA:HB2	2.02	0.94
1:A:259:GLN:HE21	1:A:284:ILE:H	0.94	0.90
1:A:152:LEU:O	1:A:155:THR:HG22	1.74	0.87

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	332/356 (93%)	304 (92%)	24 (7%)	4 (1%)	13 24
1	B	332/356 (93%)	310 (93%)	19 (6%)	3 (1%)	17 31
All	All	664/712 (93%)	614 (92%)	43 (6%)	7 (1%)	14 26

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	321	ALA
1	A	111	LYS
1	A	321	ALA
1	A	333	PRO
1	B	163	ASN

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	244/262 (93%)	223 (91%)	21 (9%)	10 20
1	B	244/262 (93%)	224 (92%)	20 (8%)	11 22
All	All	488/524 (93%)	447 (92%)	41 (8%)	11 21

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	178	GLU

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Mol	Chain	Res	Type
1	B	272	LEU
1	B	181	PHE
1	B	228	ARG
1	B	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	GLN
1	B	258	HIS
1	B	265	ASN
1	B	261	ASN
1	A	201	GLN

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 monosaccharides 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	334/356 (93%)	0.09	9 (2%)	54	58	18, 38, 58, 81	0
1	B	334/356 (93%)	0.26	18 (5%)	25	27	18, 43, 62, 79	0
All	All	668/712 (93%)	0.18	27 (4%)	38	41	18, 41, 60, 81	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.5
1	A	213	SER	4.1
1	B	159	TYR	3.9
1	B	35	HIS	3.6
1	B	42	ALA	3.6

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 monosaccharides 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.