



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 11:22 AM EDT

PDB ID : 4JAR / pdb_00004jar
Title : Crystal structure of mycobacterium tuberculosis pks11 in complex with polyketide intermediates and evidence that it synthesizes ALKYL PYRONES
Authors : Gokulan, K.; Sacchettini, J.C.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on : 2013-02-19
Resolution : 1.98 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

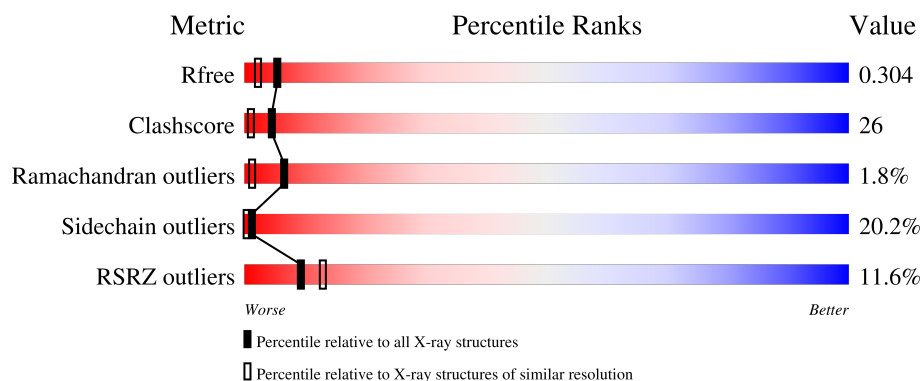
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 $\leq 5\%$. 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	353	12% 52% 34% 13% .
1	B	353	10% 56% 33% 8% .
1	C	353	10% 48% 39% 12% .
1	D	353	14% 53% 36% 10% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10576 atoms, of which 0 are hydrogens and 0 are deuteriums.

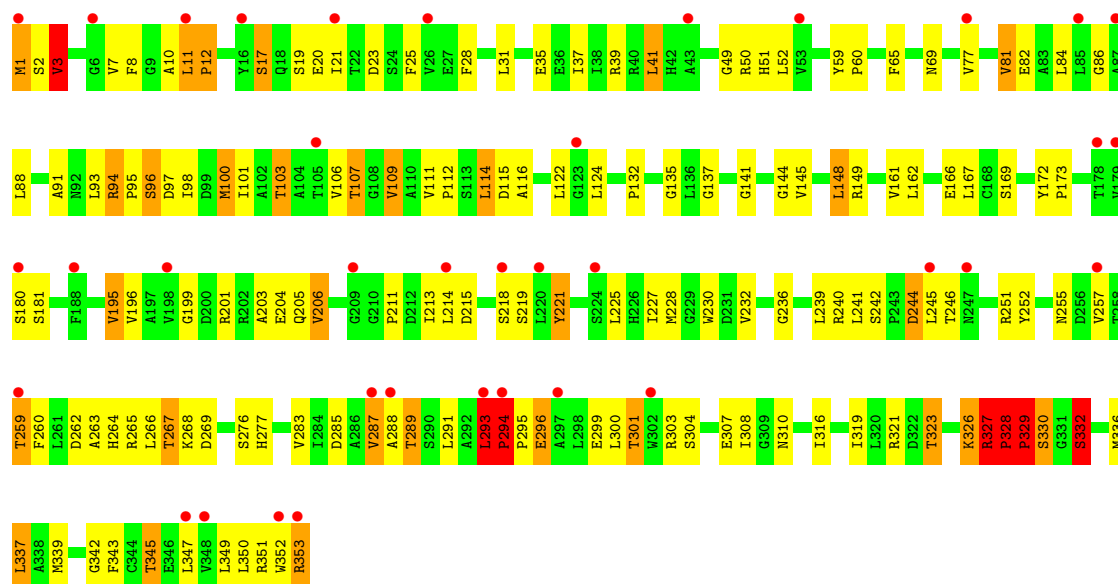
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-pyrone synthesis polyketide synthase-like Pks11.

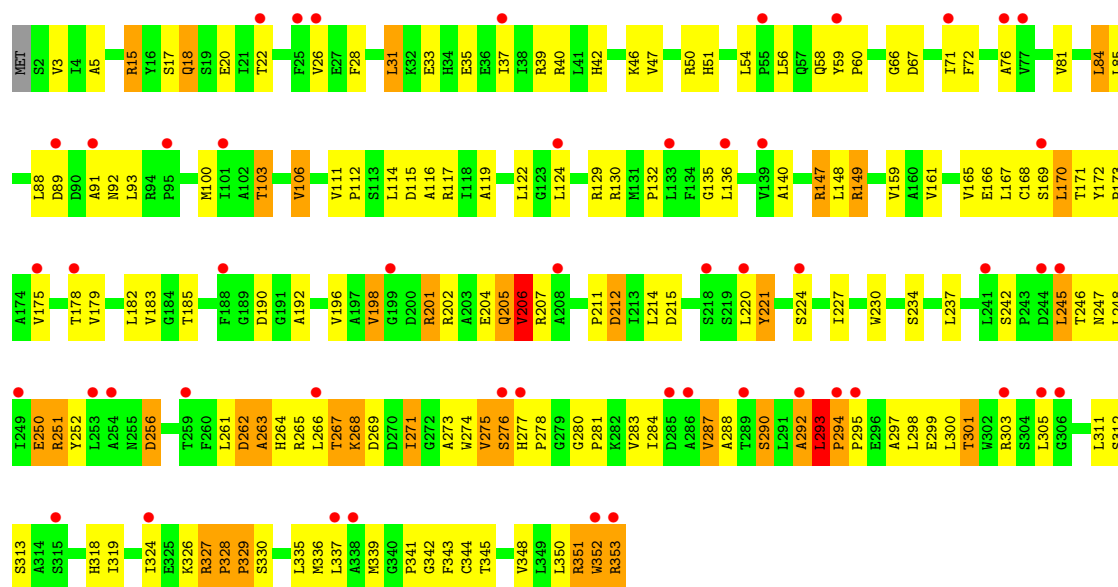
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	C	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	B	353	Total	C	N	O	S	0	0	0
			2650	1676	470	495	9			
1	D	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			



• Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11



• Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.60Å 48.52Å 195.23Å 90.00° 98.41° 90.00°	Depositor
Resolution (Å)	38.24 – 1.98 38.24 – 1.98	Depositor EDS
% Data completeness (in resolution range)	70.0 (38.24-1.98) 70.5 (38.24-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6_289)	Depositor
R, R_{free}	0.268 , 0.314 0.299 , 0.304	Depositor DCC
R_{free} test set	3377 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10576	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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, 0.333 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	0.84	2/2695 (0.1%)	1.03	10/3671 (0.3%)
1	B	0.73	5/2703 (0.2%)	1.07	13/3681 (0.4%)
1	C	0.92	8/2695 (0.3%)	1.09	12/3671 (0.3%)
1	D	0.85	8/2695 (0.3%)	1.06	12/3671 (0.3%)
All	All	0.84	23/10788 (0.2%)	1.06	47/14694 (0.3%)

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
1	B	0	1
1	C	0	1
All	All	0	3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	294	PRO	C-N	7.88	1.40	1.33
1	C	54	LEU	C-O	-7.28	1.16	1.23
1	C	205	GLN	C-N	-6.75	1.25	1.33
1	B	293	LEU	C-N	6.70	1.41	1.33
1	C	328	PRO	C-N	6.20	1.40	1.33

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	PRO	CA-C-N	-7.82	112.86	120.83
1	C	294	PRO	C-N-CA	-7.82	112.86	120.83
1	A	280	GLY	CA-C-N	7.72	127.27	119.24
1	A	280	GLY	C-N-CA	7.72	127.27	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ARG	CA-C-N	-7.51	112.64	120.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	GLY	Peptide
1	B	2	SER	Peptide
1	C	344	CYS	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	2642	0	2675	156	0
1	B	2650	0	2687	128	0
1	C	2642	0	2675	129	1
1	D	2642	0	2675	162	1
All	All	10576	0	10712	558	1

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 26.

The worst 5 of 558 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:28:PHE:HB2	1:B:31:LEU:CD1	1.46	1.44
1:C:251:ARG:HG2	1:C:252:TYR:CE1	1.59	1.38
1:A:300:LEU:CD1	1:A:323:THR:HG22	1.58	1.34
1:B:28:PHE:CB	1:B:31:LEU:HD12	1.70	1.22
1:B:84:LEU:HD23	1:B:122:LEU:CD1	1.70	1.21

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:GLU:OE1	1:D:303:ARG:NH1[1_455]	2.07	0.13

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	350/353 (99%)	319 (91%)	27 (8%)	4 (1%)	11	4
1	B	351/353 (99%)	320 (91%)	25 (7%)	6 (2%)	7	1
1	C	350/353 (99%)	304 (87%)	38 (11%)	8 (2%)	5	1
1	D	350/353 (99%)	322 (92%)	21 (6%)	7 (2%)	6	1
All	All	1401/1412 (99%)	1265 (90%)	111 (8%)	25 (2%)	6	1

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	278	PRO
1	B	330	SER
1	D	205	GLN
1	D	206	VAL
1	D	352	TRP

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	280/281 (100%)	212 (76%)	68 (24%)	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	281/281 (100%)	234 (83%)	47 (17%)	2	0
1	C	280/281 (100%)	219 (78%)	61 (22%)	1	0
1	D	280/281 (100%)	229 (82%)	51 (18%)	2	0
All	All	1121/1124 (100%)	894 (80%)	227 (20%)	1	0

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	265	ARG
1	D	301	THR
1	B	148	LEU
1	D	299	GLU
1	D	206	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	310	ASN
1	D	310	ASN
1	D	318	HIS
1	D	92	ASN
1	B	51	HIS

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 ⓘ

There are no oligosaccharides 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	352/353 (99%)	1.10	42 (11%) 9 12	24, 63, 79, 96	0
1	B	353/353 (100%)	1.06	37 (10%) 11 15	24, 61, 81, 94	0
1	C	352/353 (99%)	1.14	34 (9%) 13 19	22, 59, 83, 92	0
1	D	352/353 (99%)	1.20	51 (14%) 6 8	24, 63, 87, 96	0
All	All	1409/1412 (99%)	1.12	164 (11%) 9 13	22, 62, 83, 96	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	GLY	4.8
1	B	245	LEU	4.5
1	B	1	MET	4.5
1	C	344	CYS	4.4
1	D	292	ALA	4.4

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 oligosaccharides 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.