



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4DQV / pdb_00004dqv
Title : Crystal structure of reductase (R) domain of non-ribosomal peptide synthetase from *Mycobacterium tuberculosis*
Authors : Haque, A.S.; Panjikar, S.; Sankaranarayanan, R.
Deposited on : 2012-02-16
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

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

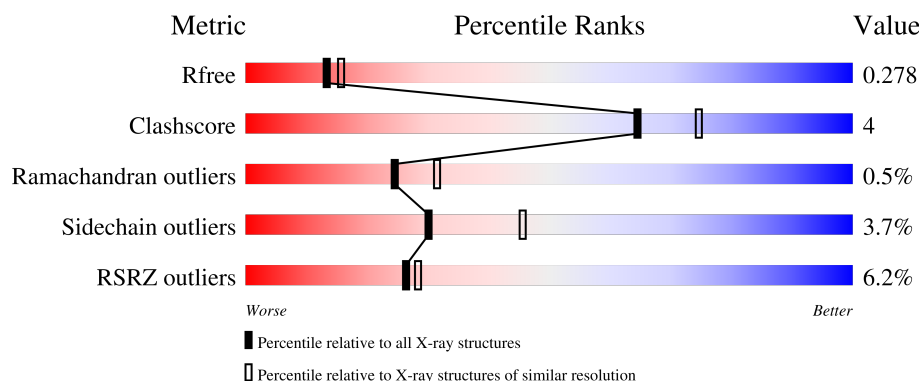
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	478	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3462 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 PROBABLE PEPTIDE SYNTHETASE NRP (PEPTIDE SYNTHASE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	Se	73	0	0
			3301	2083	579	627	4	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MSE	-	expression tag	UNP Q10896
A	-19	GLY	-	expression tag	UNP Q10896
A	-18	SER	-	expression tag	UNP Q10896
A	-17	SER	-	expression tag	UNP Q10896
A	-16	HIS	-	expression tag	UNP Q10896
A	-15	HIS	-	expression tag	UNP Q10896
A	-14	HIS	-	expression tag	UNP Q10896
A	-13	HIS	-	expression tag	UNP Q10896
A	-12	HIS	-	expression tag	UNP Q10896
A	-11	HIS	-	expression tag	UNP Q10896
A	-10	SER	-	expression tag	UNP Q10896
A	-9	SER	-	expression tag	UNP Q10896
A	-8	GLY	-	expression tag	UNP Q10896
A	-7	LEU	-	expression tag	UNP Q10896
A	-6	VAL	-	expression tag	UNP Q10896
A	-5	PRO	-	expression tag	UNP Q10896
A	-4	ARG	-	expression tag	UNP Q10896
A	-3	GLY	-	expression tag	UNP Q10896
A	-2	SER	-	expression tag	UNP Q10896
A	-1	HIS	-	expression tag	UNP Q10896
A	0	MSE	-	expression tag	UNP Q10896

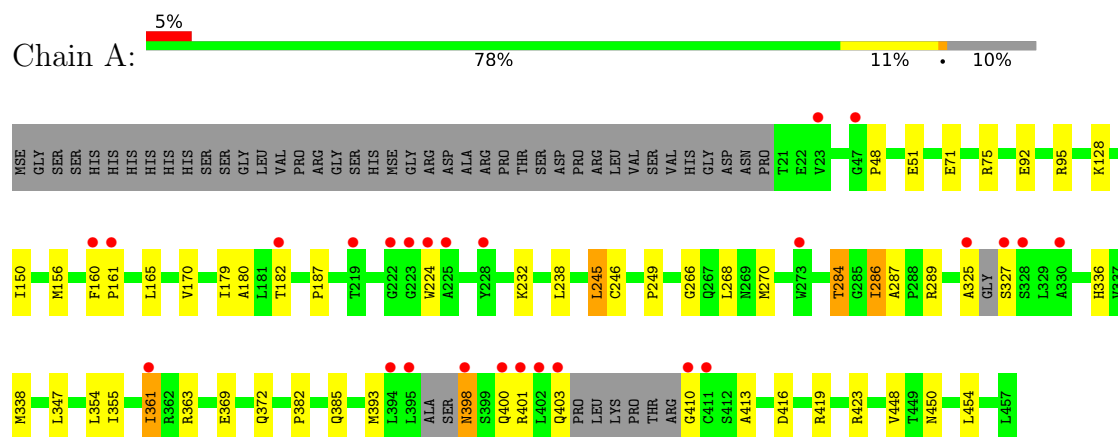
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	161	Total 161	O 161	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: PROBABLE PEPTIDE SYNTHETASE NRP (PEPTIDE SYNTHASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	59.06Å 59.06Å 238.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.15 – 2.30 51.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (51.15-2.30) 99.5 (51.15-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.278 (Not available) , 0.278	Depositor DCC
R_{free} test set	1127 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3462	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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 [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	0.65	5/3358 (0.1%)	0.91	8/4554 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TRP	CB-CG	-13.92	1.07	1.50
1	A	454	LEU	CB-CG	-9.54	1.34	1.53
1	A	95	ARG	CB-CG	-7.48	1.30	1.52
1	A	369	GLU	CB-CG	-7.18	1.30	1.52
1	A	403	GLN	CB-CG	-5.46	1.36	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	TRP	CA-CB-CG	11.68	135.79	113.60
1	A	372	GLN	CB-CG-CD	-11.03	93.84	112.60
1	A	398	ASN	CB-CG-ND2	-8.64	103.44	116.40
1	A	398	ASN	CB-CG-OD1	6.31	133.42	120.80
1	A	400	GLN	CA-CB-CG	6.20	126.50	114.10
1	A	400	GLN	CB-CG-CD	6.12	123.00	112.60
1	A	182	THR	N-CA-C	5.90	118.85	111.24
1	A	286	ILE	N-CA-C	5.07	115.21	108.11

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	3301	0	3267	25	0
2	A	161	0	0	2	0
All	All	3462	0	3267	25	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 4.

All (25) 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:A:284:THR:HG23	1:A:286:ILE:H	1.47	0.80
1:A:325:ALA:C	1:A:327:SER:O	2.36	0.69
1:A:410:GLY:N	2:A:542:HOH:O	2.28	0.67
1:A:338:MSE:HE1	1:A:413:ALA:HB3	1.80	0.62
1:A:336:HIS:HB3	1:A:338:MSE:HE2	1.83	0.61
1:A:382:PRO:HD2	1:A:385:GLN:HE21	1.65	0.60
1:A:48:PRO:HG2	1:A:249:PRO:HG2	1.86	0.57
1:A:289:ARG:HH11	1:A:289:ARG:HB3	1.70	0.55
1:A:355:ILE:HG12	1:A:361:ILE:HG23	1.89	0.54
1:A:150:ILE:HD12	1:A:180:ALA:HB2	1.92	0.51
1:A:170:VAL:HG13	1:A:238:LEU:HD11	1.92	0.50
1:A:287:ALA:O	1:A:363:ARG:HA	2.13	0.49
1:A:268:LEU:HD23	1:A:270:MSE:HE1	1.94	0.49
1:A:266:GLY:H	1:A:450:ASN:ND2	2.11	0.48
1:A:382:PRO:HD2	1:A:385:GLN:NE2	2.28	0.48
1:A:48:PRO:HB3	1:A:187:PRO:HD3	1.95	0.48
1:A:71:GLU:O	1:A:75:ARG:HG2	2.16	0.46
1:A:419:ARG:O	1:A:423:ARG:HG3	2.17	0.45
1:A:289:ARG:HB3	1:A:289:ARG:NH1	2.32	0.44
1:A:268:LEU:HD22	1:A:450:ASN:HB3	2.00	0.43
1:A:245:LEU:HB3	1:A:246:CYS:SG	2.59	0.43
1:A:128:LYS:HE3	2:A:562:HOH:O	2.19	0.43
1:A:287:ALA:HB2	1:A:361:ILE:HD11	2.01	0.42
1:A:160:PHE:HB3	1:A:161:PRO:HD3	2.02	0.42
1:A:232:LYS:HA	1:A:232:LYS:HD3	1.91	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	420/478 (88%)	402 (96%)	16 (4%)	2 (0%)	24	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	ARG
1	A	393	MSE

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	348/380 (92%)	335 (96%)	13 (4%)	30	45

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

Mol	Chain	Res	Type
1	A	51	GLU
1	A	92	GLU
1	A	156	MSE
1	A	165	LEU
1	A	179	ILE
1	A	245	LEU
1	A	284	THR
1	A	347	LEU
1	A	354	LEU

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Mol	Chain	Res	Type
1	A	361	ILE
1	A	398	ASN
1	A	416	ASP
1	A	448	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	163	HIS
1	A	269	ASN
1	A	385	GLN
1	A	438	HIS
1	A	450	ASN

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 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

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	420/478 (87%)	0.38	26 (6%)	26 28	21, 42, 62, 82	15 (3%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	LEU	4.9
1	A	222	GLY	4.6
1	A	224	TRP	4.4
1	A	325	ALA	4.3
1	A	400	GLN	4.2
1	A	160	PHE	4.0
1	A	161	PRO	3.7
1	A	328	SER	3.4
1	A	330	ALA	3.3
1	A	411	CYS	3.2
1	A	403	GLN	3.2
1	A	401	ARG	2.9
1	A	395	LEU	2.7
1	A	398	ASN	2.7
1	A	402	LEU	2.7
1	A	223	GLY	2.5
1	A	273	TRP	2.4
1	A	182	THR	2.4
1	A	327	SER	2.3
1	A	361	ILE	2.3
1	A	228	TYR	2.1
1	A	410	GLY	2.1
1	A	23	VAL	2.1
1	A	47	GLY	2.0
1	A	219	THR	2.0
1	A	225	ALA	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 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.