



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2UYO / pdb_00002uyo
Title : Crystal structure of ML2640c from Mycobacterium leprae in an hexagonal crystal form
Authors : Grana, M.; Buschiazzo, A.; Wehenkel, A.; Haouz, A.; Miras, I.; Shepard, W.; Alzari, P.M.
Deposited on : 2007-04-11
Resolution : 1.70 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
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

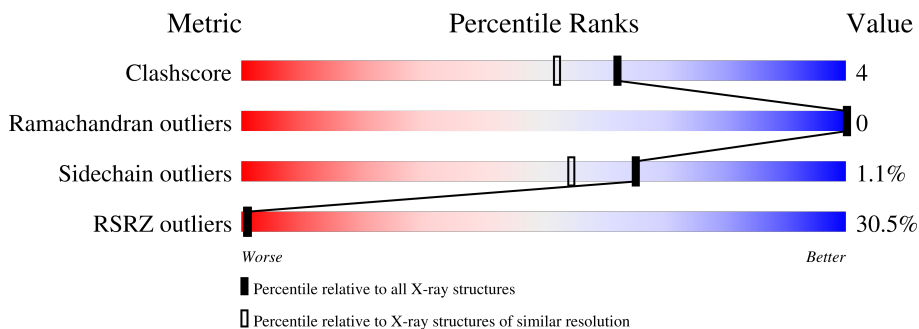
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	310	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2261 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 HYPOTHETICAL PROTEIN ML2640.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2050	1290	371	384	5			

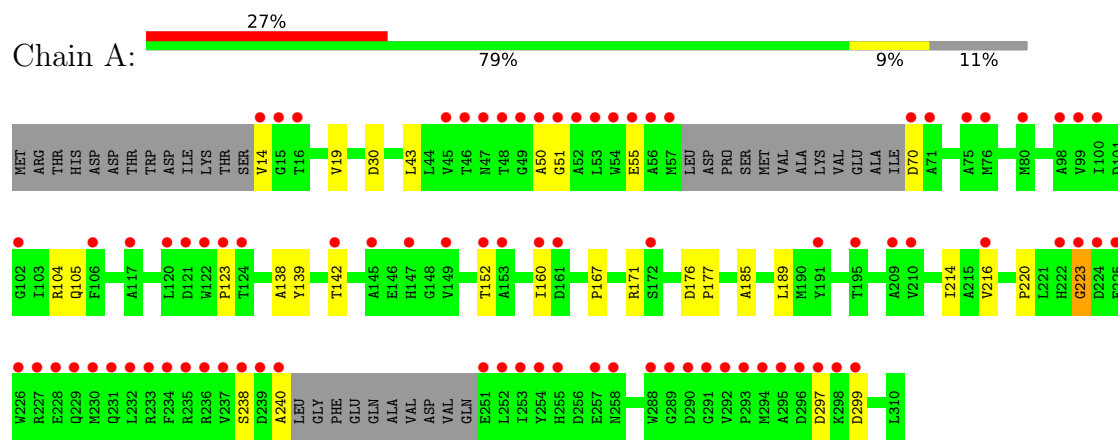
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	211	Total	O	0	0
			211	211		

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: HYPOTHETICAL PROTEIN ML2640



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	75.72Å 75.72Å 105.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.51 – 1.70 65.51 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (65.51-1.70) 99.2 (65.51-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.234 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2261	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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	1.03	2/2098 (0.1%)	0.97	2/2869 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	ASP	CG-OD1	10.19	1.44	1.25
1	A	70	ASP	CB-CG	5.64	1.66	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	GLY	N-CA-C	5.45	126.09	113.18
1	A	167	PRO	N-CA-C	5.18	117.02	110.70

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	2050	0	1901	16	0
2	A	211	0	0	2	1
All	All	2261	0	1901	16	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 4.

All (16) 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:105:GLN:HE22	1:A:176:ASP:H	1.34	0.74
1:A:51:GLY:O	1:A:55:GLU:CB	2.39	0.70
1:A:152:THR:HG23	2:A:2079:HOH:O	1.99	0.61
1:A:185:ALA:HB3	1:A:216:VAL:HG22	1.83	0.59
1:A:189:LEU:HD11	1:A:216:VAL:HG11	1.93	0.50
1:A:214:ILE:HG12	1:A:216:VAL:HG23	1.95	0.49
1:A:43:LEU:HG	2:A:2029:HOH:O	2.13	0.48
1:A:220:PRO:HB2	1:A:223:GLY:HA3	1.96	0.46
1:A:138:ALA:O	1:A:142:THR:HG23	2.15	0.46
1:A:105:GLN:NE2	1:A:176:ASP:H	2.07	0.46
1:A:19:VAL:HG11	1:A:50:ALA:HB3	1.97	0.46
1:A:14:VAL:HG21	1:A:139:TYR:CD2	2.51	0.46
1:A:297:ASP:OD1	1:A:299:ASP:HB2	2.18	0.44
1:A:104:ARG:CZ	1:A:123:PRO:HG2	2.51	0.41
1:A:171:ARG:NH1	1:A:177:PRO:HG2	2.35	0.41
1:A:238:SER:C	1:A:240:ALA:H	2.29	0.41

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)
2:A:2177:HOH:O	2:A:2196:HOH:O[6_564]	2.13	0.07

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	269/310 (87%)	261 (97%)	8 (3%)	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	189/247 (76%)	187 (99%)	2 (1%)	65 54

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	160	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	105	GLN
1	A	133	GLN
1	A	197	GLN
1	A	255	HIS

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

There are no ligands in this entry.

5.7 Other polymers

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

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	275/310 (88%)	1.90	84 (30%) 1 1	20, 27, 50, 56	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	GLU	8.8
1	A	293	PRO	8.5
1	A	48	THR	8.4
1	A	226	TRP	7.4
1	A	227	ARG	7.2
1	A	237	VAL	7.1
1	A	292	VAL	6.7
1	A	236	ARG	6.7
1	A	52	ALA	6.4
1	A	238	SER	6.4
1	A	224	ASP	6.2
1	A	252	LEU	6.0
1	A	49	GLY	5.8
1	A	50	ALA	5.7
1	A	54	TRP	5.7
1	A	240	ALA	5.3
1	A	229	GLN	5.3
1	A	296	ASP	5.2
1	A	70	ASP	5.2
1	A	232	LEU	5.2
1	A	239	ASP	5.1
1	A	71	ALA	5.1
1	A	297	ASP	4.9
1	A	51	GLY	4.8
1	A	223	GLY	4.7
1	A	228	GLU	4.7
1	A	14	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	80	MET	4.6
1	A	234	PHE	4.6
1	A	47	ASN	4.2
1	A	290	ASP	4.2
1	A	295	ALA	4.1
1	A	230	MET	4.1
1	A	56	ALA	4.1
1	A	235	ARG	4.0
1	A	294	MET	4.0
1	A	291	GLY	3.8
1	A	153	ALA	3.7
1	A	258	ASN	3.5
1	A	251	GLU	3.5
1	A	46	THR	3.4
1	A	124	THR	3.4
1	A	231	GLN	3.3
1	A	16	THR	3.3
1	A	142	THR	3.3
1	A	210	VAL	3.3
1	A	149	VAL	3.3
1	A	298	LYS	3.2
1	A	233	ARG	3.1
1	A	195	THR	3.1
1	A	253	ILE	3.0
1	A	57	MET	3.0
1	A	288	TRP	2.9
1	A	121	ASP	2.9
1	A	222	HIS	2.9
1	A	98	ALA	2.8
1	A	55	GLU	2.8
1	A	76	MET	2.8
1	A	257	GLU	2.8
1	A	53	LEU	2.8
1	A	122	TRP	2.8
1	A	289	GLY	2.8
1	A	99	VAL	2.8
1	A	216	VAL	2.6
1	A	147	HIS	2.6
1	A	123	PRO	2.6
1	A	161	ASP	2.5
1	A	145	ALA	2.5
1	A	106	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	15	GLY	2.5
1	A	117	ALA	2.5
1	A	172	SER	2.4
1	A	152	THR	2.4
1	A	254	TYR	2.4
1	A	160	ILE	2.4
1	A	120	LEU	2.3
1	A	100	ILE	2.3
1	A	191	TYR	2.3
1	A	75	ALA	2.3
1	A	255	HIS	2.3
1	A	45	VAL	2.3
1	A	209	ALA	2.2
1	A	299	ASP	2.1
1	A	102	GLY	2.1

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.