



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 09:23 AM GMT

PDB ID : 1TM0
Title : Crystal Structure of the putative proline racemase from Brucella melitensis,
Northeast Structural Genomics Target LR31
Authors : Forouhar, F.; Chen, Y.; Xiao, R.; Ho, C.K.; Ma, L.-C.; Cooper, B.; Acton,
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Consortium (NESG)
Deposited on : 2004-06-10
Resolution : 2.80 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>

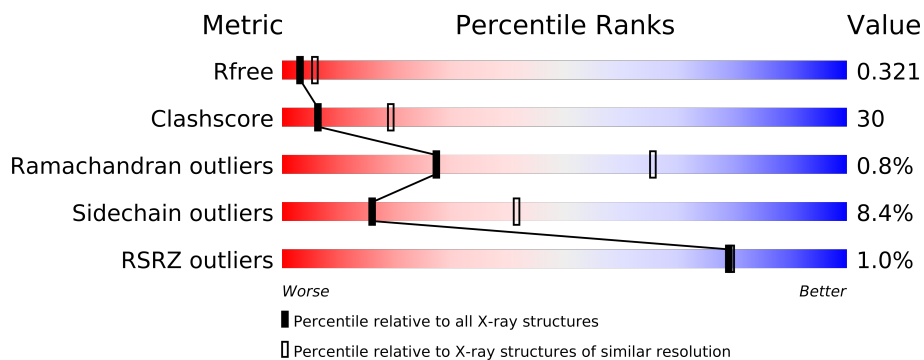
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	350	
1	B	350	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4718 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 PROLINE RACEMASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	Se	0	0	0
			2342	1471	416	439	6	10			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2342	1471	416	439	6	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	76	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	81	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	89	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	116	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	164	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	263	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	272	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	321	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
A	343	LEU	-	CLONING ARTIFACT	UNP Q8YFD6
A	344	GLU	-	CLONING ARTIFACT	UNP Q8YFD6
A	345	HIS	-	EXPRESSION TAG	UNP Q8YFD6
A	346	HIS	-	EXPRESSION TAG	UNP Q8YFD6
A	347	HIS	-	EXPRESSION TAG	UNP Q8YFD6
A	348	HIS	-	EXPRESSION TAG	UNP Q8YFD6
A	349	HIS	-	EXPRESSION TAG	UNP Q8YFD6
A	350	HIS	-	EXPRESSION TAG	UNP Q8YFD6
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	76	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	81	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	89	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	109	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	116	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	164	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	263	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	272	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	321	MSE	MET	MODIFIED RESIDUE	UNP Q8YFD6
B	343	LEU	-	CLONING ARTIFACT	UNP Q8YFD6
B	344	GLU	-	CLONING ARTIFACT	UNP Q8YFD6
B	345	HIS	-	EXPRESSION TAG	UNP Q8YFD6
B	346	HIS	-	EXPRESSION TAG	UNP Q8YFD6
B	347	HIS	-	EXPRESSION TAG	UNP Q8YFD6
B	348	HIS	-	EXPRESSION TAG	UNP Q8YFD6
B	349	HIS	-	EXPRESSION TAG	UNP Q8YFD6
B	350	HIS	-	EXPRESSION TAG	UNP Q8YFD6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	23	Total O 23 23	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.03Å 77.36Å 77.42Å 90.00° 124.11° 90.00°	Depositor
Resolution (Å)	28.57 – 2.80 28.57 – 2.84	Depositor EDS
% Data completeness (in resolution range)	84.3 (28.57-2.80) 91.5 (28.57-2.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.312 0.252 , 0.321	Depositor DCC
R_{free} test set	1371 reflections (9.37%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , -0.7	EDS
Estimated twinning fraction	0.015 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.015 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.016 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.014 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.014 for $-h+k-l, -l, -k$ 0.015 for $-h-k-l, l, k$ 0.015 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.014 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.016 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.016 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.469 for $-h-2^*l, -k, l$	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29250 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4718	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

¹Intensities estimated from amplitudes.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.42	0/2379	0.61	0/3209
1	B	0.44	0/2379	0.63	0/3209
All	All	0.43	0/4758	0.62	0/6418

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2342	0	2344	134	0
1	B	2342	0	2344	151	0
2	A	11	0	0	1	0
2	B	23	0	0	4	0
All	All	4718	0	4688	283	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 30.

The worst 5 of 283 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:ASN:HD22	1:A:144:VAL:N	1.50	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:143:ASN:HD22	1:B:144:VAL:N	1.50	1.08
1:A:143:ASN:ND2	1:A:144:VAL:H	1.56	1.02
1:B:143:ASN:ND2	1:B:144:VAL:H	1.57	1.02
1:B:308:ILE:H	1:B:308:ILE:HD12	1.23	1.01

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	301/350 (86%)	264 (88%)	36 (12%)	1 (0%)	50	84
1	B	301/350 (86%)	264 (88%)	33 (11%)	4 (1%)	18	51
All	All	602/700 (86%)	528 (88%)	69 (12%)	5 (1%)	27	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	THR
1	A	215	GLU
1	B	215	GLU
1	B	217	ASP
1	B	281	LYS

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	255/279 (91%)	235 (92%)	20 (8%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	255/279 (91%)	232 (91%)	23 (9%)	14	37
All	All	510/558 (91%)	467 (92%)	43 (8%)	16	41

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
1	B	89	MSE
1	B	297	GLU
1	B	1	MSE
1	B	13	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
1	B	13	HIS
1	B	143	ASN
1	A	225	GLN
1	B	181	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	311/350 (88%)	-0.14	3 (0%) 79 79	4, 29, 65, 78	0
1	B	311/350 (88%)	-0.18	3 (0%) 79 79	5, 28, 67, 77	0
All	All	622/700 (88%)	-0.16	6 (0%) 79 79	4, 29, 66, 78	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	PRO	5.3
1	A	204	ALA	5.0
1	B	256	GLY	2.8
1	A	254	PRO	2.6
1	B	163	ILE	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.