



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:04 AM GMT

PDB ID : 3H12
Title : Crystal structure of putative mandelate racemase from Bordetella Bronchiseptica RB50
Authors : Malashkevich, V.N.; Toro, R.; Morano, C.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-04-10
Resolution : 1.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

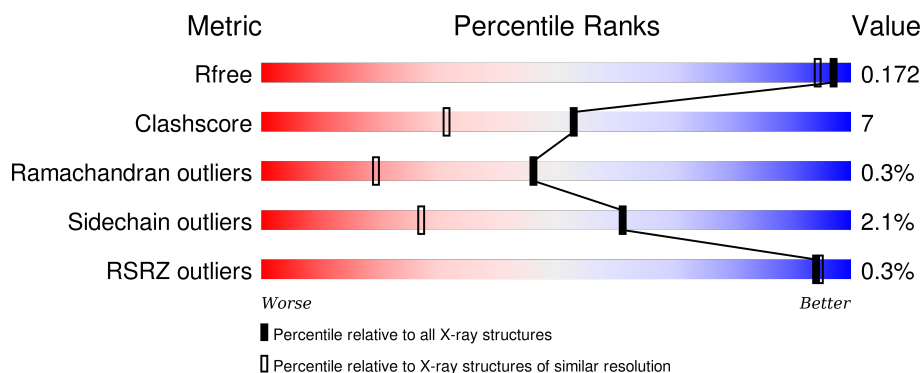
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	397	 83% 14% ..
1	B	397	 83% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6853 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 mandelate racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	2	0
			3029	1908	553	558	10			
1	B	392	Total	C	N	O	S	0	3	0
			3041	1917	554	560	10			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q7WEE8
A	2	SER	-	expression tag	UNP Q7WEE8
A	3	LEU	-	expression tag	UNP Q7WEE8
A	390	GLU	-	expression tag	UNP Q7WEE8
A	391	GLY	-	expression tag	UNP Q7WEE8
A	392	HIS	-	expression tag	UNP Q7WEE8
A	393	HIS	-	expression tag	UNP Q7WEE8
A	394	HIS	-	expression tag	UNP Q7WEE8
A	395	HIS	-	expression tag	UNP Q7WEE8
A	396	HIS	-	expression tag	UNP Q7WEE8
A	397	HIS	-	expression tag	UNP Q7WEE8
B	1	MET	-	expression tag	UNP Q7WEE8
B	2	SER	-	expression tag	UNP Q7WEE8
B	3	LEU	-	expression tag	UNP Q7WEE8
B	390	GLU	-	expression tag	UNP Q7WEE8
B	391	GLY	-	expression tag	UNP Q7WEE8
B	392	HIS	-	expression tag	UNP Q7WEE8
B	393	HIS	-	expression tag	UNP Q7WEE8
B	394	HIS	-	expression tag	UNP Q7WEE8
B	395	HIS	-	expression tag	UNP Q7WEE8
B	396	HIS	-	expression tag	UNP Q7WEE8
B	397	HIS	-	expression tag	UNP Q7WEE8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Na 1	0	0
2	A	1	Total 1	Na 1	0	0

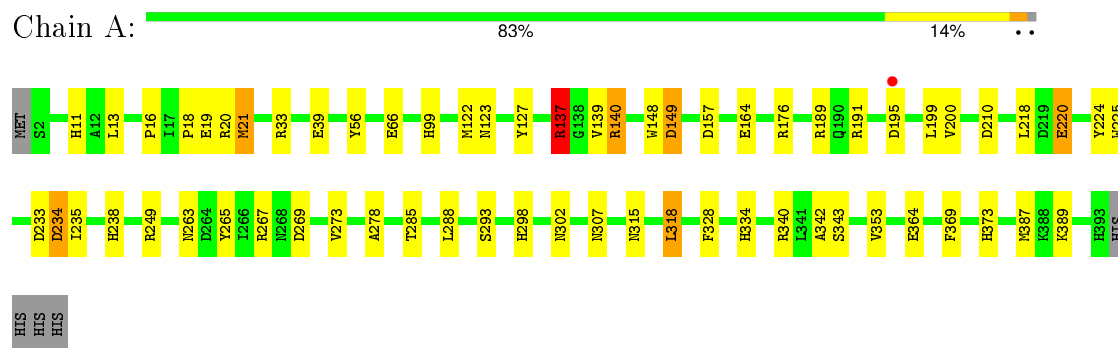
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	386	Total 386	O 386	0	0
3	B	395	Total 395	O 395	0	0

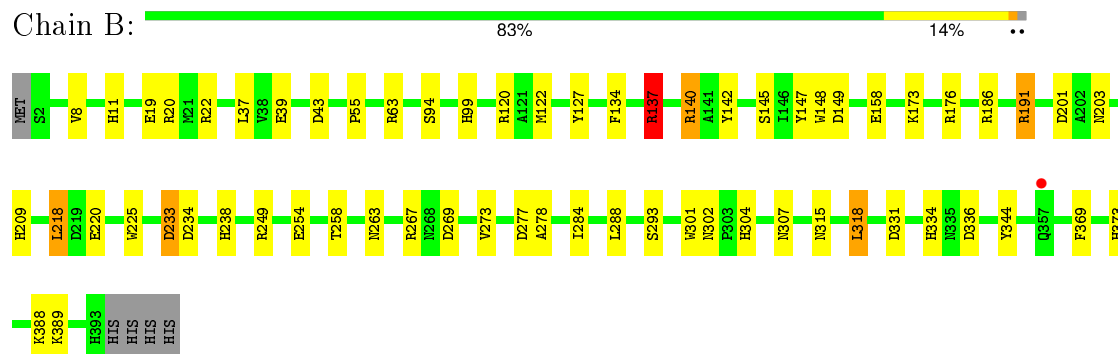
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: mandelate racemase



- Molecule 1: mandelate racemase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	116.15Å 116.15Å 128.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.73 – 1.50 8.73 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (8.73-1.50) 95.8 (8.73-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.146 , 0.173 0.145 , 0.172	Depositor DCC
R_{free} test set	6483 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 51.9	EDS
Estimated twinning fraction	0.023 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 128901 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6853	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	1.49	10/3104 (0.3%)	1.34	27/4216 (0.6%)
1	B	1.47	20/3117 (0.6%)	1.33	26/4234 (0.6%)
All	All	1.48	30/6221 (0.5%)	1.34	53/8450 (0.6%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	MET	CB-CG	12.67	1.92	1.51
1	A	21	MET	CG-SD	10.51	2.08	1.81
1	B	220	GLU	CG-CD	8.89	1.65	1.51
1	B	19	GLU	CB-CG	-8.38	1.36	1.52
1	A	293	SER	CB-OG	7.51	1.52	1.42

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	MET	CB-CG-SD	-10.29	81.52	112.40
1	B	176	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	A	218	LEU	CB-CG-CD2	9.00	126.30	111.00
1	A	176	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	249	ARG	NE-CZ-NH1	8.24	124.42	120.30

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	3029	0	2990	50	0
1	B	3041	0	2998	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	386	0	0	15	4
3	B	395	0	0	16	4
All	All	6853	0	5988	80	4

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 7.

The worst 5 of 80 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:21:MET:CG	1:A:21:MET:CB	1.91	1.45
1:A:21:MET:CG	1:A:21:MET:SD	2.08	1.41
1:A:364:GLU:HB2	3:A:537:HOH:O	1.27	1.30
1:A:21:MET:HG2	3:A:749:HOH:O	1.51	1.11
1:A:288:LEU:HD23	1:A:318:LEU:HD21	1.29	1.07

All (4) 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)
3:A:732:HOH:O	3:B:482:HOH:O[3_655]	2.04	0.16
3:A:715:HOH:O	3:B:890:HOH:O[6_555]	2.09	0.11
3:A:622:HOH:O	3:B:623:HOH:O[3_655]	2.12	0.08
3:A:461:HOH:O	3:B:834:HOH:O[3_655]	2.14	0.06

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	392/397 (99%)	375 (96%)	16 (4%)	1 (0%)	46	19
1	B	393/397 (99%)	380 (97%)	12 (3%)	1 (0%)	46	19
All	All	785/794 (99%)	755 (96%)	28 (4%)	2 (0%)	46	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	B	307	ASN

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	307/310 (99%)	299 (97%)	8 (3%)	54	19
1	B	308/310 (99%)	303 (98%)	5 (2%)	70	41
All	All	615/620 (99%)	602 (98%)	13 (2%)	61	27

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	TRP
1	A	318	LEU
1	B	218	LEU
1	A	140	ARG
1	B	140	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	99	HIS
1	B	209	HIS

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Mol	Chain	Res	Type
1	B	334	HIS
1	B	123	ASN
1	B	203	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	392/397 (98%)	-0.69	1 (0%) 94 95	13, 17, 30, 53	0
1	B	392/397 (98%)	-0.73	1 (0%) 94 95	14, 17, 29, 50	0
All	All	784/794 (98%)	-0.71	2 (0%) 94 95	13, 17, 30, 53	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	GLN	2.2
1	A	195	ASP	2.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NA	A	500	1/1	1.00	0.03	-2.53	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NA	B	500	1/1	1.00	0.02	-3.08	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.