



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:26 pm GMT

PDB ID : 3RH9
Title : The crystal structure of oxidoreductase from *Marinobacter aquaeolei*
Authors : Zhang, Z.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on : 2011-04-11
Resolution : 2.63 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

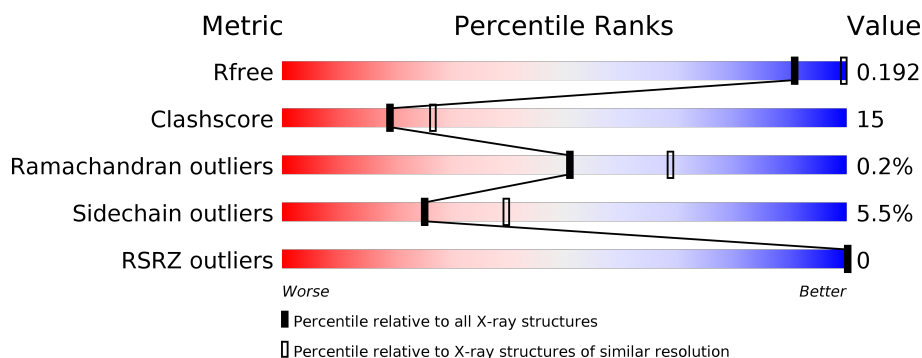
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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}	100719	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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	506	
1	B	506	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7507 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 Succinate-semialdehyde dehydrogenase (NAD(P)(+)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	Se	0	0	0
			3636	2306	620	687	9	14			
1	B	476	Total	C	N	O	S	Se	0	0	0
			3612	2292	615	682	9	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	EXPRESSION TAG	UNP A1U6U7
A	0	VAL	-	EXPRESSION TAG	UNP A1U6U7
A	483	ALA	-	EXPRESSION TAG	UNP A1U6U7
A	484	GLU	-	EXPRESSION TAG	UNP A1U6U7
A	485	ASN	-	EXPRESSION TAG	UNP A1U6U7
A	486	LEU	-	EXPRESSION TAG	UNP A1U6U7
A	487	TYR	-	EXPRESSION TAG	UNP A1U6U7
A	488	PHE	-	EXPRESSION TAG	UNP A1U6U7
A	489	GLN	-	EXPRESSION TAG	UNP A1U6U7
A	490	SER	-	EXPRESSION TAG	UNP A1U6U7
A	491	HIS	-	EXPRESSION TAG	UNP A1U6U7
A	492	HIS	-	EXPRESSION TAG	UNP A1U6U7
A	493	HIS	-	EXPRESSION TAG	UNP A1U6U7
A	494	HIS	-	EXPRESSION TAG	UNP A1U6U7
A	495	HIS	-	EXPRESSION TAG	UNP A1U6U7
A	496	HIS	-	EXPRESSION TAG	UNP A1U6U7
A	497	TRP	-	EXPRESSION TAG	UNP A1U6U7
A	498	SER	-	EXPRESSION TAG	UNP A1U6U7
A	499	HIS	-	EXPRESSION TAG	UNP A1U6U7
A	500	PRO	-	EXPRESSION TAG	UNP A1U6U7
A	501	GLN	-	EXPRESSION TAG	UNP A1U6U7
A	502	PHE	-	EXPRESSION TAG	UNP A1U6U7
A	503	GLU	-	EXPRESSION TAG	UNP A1U6U7
A	504	LYS	-	EXPRESSION TAG	UNP A1U6U7
B	-1	MSE	-	EXPRESSION TAG	UNP A1U6U7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	VAL	-	EXPRESSION TAG	UNP A1U6U7
B	483	ALA	-	EXPRESSION TAG	UNP A1U6U7
B	484	GLU	-	EXPRESSION TAG	UNP A1U6U7
B	485	ASN	-	EXPRESSION TAG	UNP A1U6U7
B	486	LEU	-	EXPRESSION TAG	UNP A1U6U7
B	487	TYR	-	EXPRESSION TAG	UNP A1U6U7
B	488	PHE	-	EXPRESSION TAG	UNP A1U6U7
B	489	GLN	-	EXPRESSION TAG	UNP A1U6U7
B	490	SER	-	EXPRESSION TAG	UNP A1U6U7
B	491	HIS	-	EXPRESSION TAG	UNP A1U6U7
B	492	HIS	-	EXPRESSION TAG	UNP A1U6U7
B	493	HIS	-	EXPRESSION TAG	UNP A1U6U7
B	494	HIS	-	EXPRESSION TAG	UNP A1U6U7
B	495	HIS	-	EXPRESSION TAG	UNP A1U6U7
B	496	HIS	-	EXPRESSION TAG	UNP A1U6U7
B	497	TRP	-	EXPRESSION TAG	UNP A1U6U7
B	498	SER	-	EXPRESSION TAG	UNP A1U6U7
B	499	HIS	-	EXPRESSION TAG	UNP A1U6U7
B	500	PRO	-	EXPRESSION TAG	UNP A1U6U7
B	501	GLN	-	EXPRESSION TAG	UNP A1U6U7
B	502	PHE	-	EXPRESSION TAG	UNP A1U6U7
B	503	GLU	-	EXPRESSION TAG	UNP A1U6U7
B	504	LYS	-	EXPRESSION TAG	UNP A1U6U7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	119	Total O 119 119	0	0
2	B	140	Total O 140 140	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.48Å 102.48Å 144.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 2.63 49.32 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.32-2.63) 99.8 (49.32-2.63)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.14 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.187 , 0.252 0.186 , 0.192	Depositor DCC
R_{free} test set	1537 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7507	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.46	0/3702	0.57	0/4994
1	B	0.52	1/3677 (0.0%)	0.58	0/4959
All	All	0.49	1/7379 (0.0%)	0.58	0/9953

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	PHE	CD1-CE1	-5.40	1.28	1.39

There are no bond angle outliers.

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	3636	0	3601	106	0
1	B	3612	0	3580	105	0
2	A	119	0	0	2	0
2	B	140	0	0	2	0
All	All	7507	0	7181	210	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 15.

The worst 5 of 210 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:287:THR:HG22	1:A:289:VAL:H	1.21	1.02
1:B:287:THR:HG22	1:B:289:VAL:H	1.27	0.97
1:B:222:HIS:HD2	1:B:224:ASP:H	1.17	0.90
1:B:96:GLU:HG3	1:B:184:THR:HG22	1.55	0.89
1:A:279:ASN:HD21	1:A:291:ALA:H	1.19	0.88

There are no symmetry-related clashes.

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	479/506 (95%)	461 (96%)	18 (4%)	0	100	100
1	B	472/506 (93%)	450 (95%)	20 (4%)	2 (0%)	38	54
All	All	951/1012 (94%)	911 (96%)	38 (4%)	2 (0%)	51	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	LYS
1	B	413	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/389 (97%)	358 (94%)	21 (6%)	25	40
1	B	378/389 (97%)	357 (94%)	21 (6%)	25	39
All	All	757/778 (97%)	715 (94%)	42 (6%)	25	40

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	THR
1	B	20	ASP
1	B	380	MSE
1	A	434	ARG
1	B	6	LEU

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

Mol	Chain	Res	Type
1	A	408	ASN
1	B	57	GLN
1	B	292	ASN
1	A	384	GLN
1	B	384	GLN

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](#)

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	467/506 (92%)	-0.56	0 100 100	10, 18, 27, 39	0
1	B	462/506 (91%)	-0.61	0 100 100	10, 16, 23, 41	0
All	All	929/1012 (91%)	-0.58	0 100 100	10, 17, 25, 41	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.