



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 03:28 PM GMT

PDB ID : 3L6E
Title : Crystal structure of putative short chain dehydrogenase/reductasefamily oxidoreductase from Aeromonas hydrophila subsp. hydrophila ATCC 7966
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Deposited on : 2009-12-23
Resolution : 2.30 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>

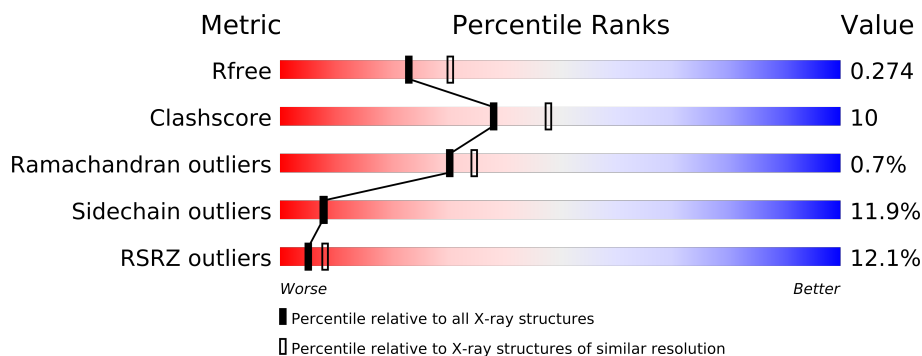
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 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	235	
1	B	235	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	500	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3296 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 Oxidoreductase, short-chain dehydrogenase/reductasefamily.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	Se	0	0	0
			1585	993	287	296	3	6			
1	B	210	Total	C	N	O	S	Se	0	0	0
			1594	1000	287	298	3	6			

There are 48 discrepancies between the modelled and reference sequences:

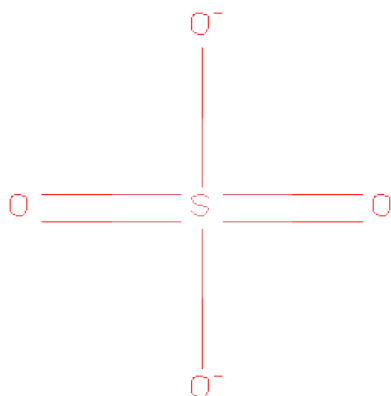
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP A0KPA6
A	2	SER	-	EXPRESSION TAG	UNP A0KPA6
A	3	LEU	-	EXPRESSION TAG	UNP A0KPA6
A	42	GLN	GLU	CONFLICT	UNP A0KPA6
A	45	LEU	GLU	CONFLICT	UNP A0KPA6
A	49	ASN	LYS	CONFLICT	UNP A0KPA6
A	55	VAL	ALA	CONFLICT	UNP A0KPA6
A	63	ASP	GLU	CONFLICT	UNP A0KPA6
A	87	THR	VAL	CONFLICT	UNP A0KPA6
A	105	MSE	VAL	CONFLICT	UNP A0KPA6
A	110	VAL	ILE	CONFLICT	UNP A0KPA6
A	125	GLU	ASP	CONFLICT	UNP A0KPA6
A	126	ARG	LYS	CONFLICT	UNP A0KPA6
A	168	ASP	GLY	CONFLICT	UNP A0KPA6
A	189	THR	SER	CONFLICT	UNP A0KPA6
A	194	PRO	SER	CONFLICT	UNP A0KPA6
A	228	GLU	-	EXPRESSION TAG	UNP A0KPA6
A	229	GLY	-	EXPRESSION TAG	UNP A0KPA6
A	230	HIS	-	EXPRESSION TAG	UNP A0KPA6
A	231	HIS	-	EXPRESSION TAG	UNP A0KPA6
A	232	HIS	-	EXPRESSION TAG	UNP A0KPA6
A	233	HIS	-	EXPRESSION TAG	UNP A0KPA6
A	234	HIS	-	EXPRESSION TAG	UNP A0KPA6
A	235	HIS	-	EXPRESSION TAG	UNP A0KPA6
B	1	MSE	-	EXPRESSION TAG	UNP A0KPA6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	EXPRESSION TAG	UNP A0KPA6
B	3	LEU	-	EXPRESSION TAG	UNP A0KPA6
B	42	GLN	GLU	CONFLICT	UNP A0KPA6
B	45	LEU	GLU	CONFLICT	UNP A0KPA6
B	49	ASN	LYS	CONFLICT	UNP A0KPA6
B	55	VAL	ALA	CONFLICT	UNP A0KPA6
B	63	ASP	GLU	CONFLICT	UNP A0KPA6
B	87	THR	VAL	CONFLICT	UNP A0KPA6
B	105	MSE	VAL	CONFLICT	UNP A0KPA6
B	110	VAL	ILE	CONFLICT	UNP A0KPA6
B	125	GLU	ASP	CONFLICT	UNP A0KPA6
B	126	ARG	LYS	CONFLICT	UNP A0KPA6
B	168	ASP	GLY	CONFLICT	UNP A0KPA6
B	189	THR	SER	CONFLICT	UNP A0KPA6
B	194	PRO	SER	CONFLICT	UNP A0KPA6
B	228	GLU	-	EXPRESSION TAG	UNP A0KPA6
B	229	GLY	-	EXPRESSION TAG	UNP A0KPA6
B	230	HIS	-	EXPRESSION TAG	UNP A0KPA6
B	231	HIS	-	EXPRESSION TAG	UNP A0KPA6
B	232	HIS	-	EXPRESSION TAG	UNP A0KPA6
B	233	HIS	-	EXPRESSION TAG	UNP A0KPA6
B	234	HIS	-	EXPRESSION TAG	UNP A0KPA6
B	235	HIS	-	EXPRESSION TAG	UNP A0KPA6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	63	Total	O	0	0
			63	63		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.36Å 53.01Å 67.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 35.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.30) 97.7 (35.86-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.02 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.219 , 0.270 0.228 , 0.274	Depositor DCC
R_{free} test set	1031 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 20490 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3296	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.53	0/1600	0.63	0/2150
1	B	0.59	0/1610	0.67	1/2163 (0.0%)
All	All	0.56	0/3210	0.65	1/4313 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	LEU	CB-CG-CD1	-5.16	102.22	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	36	ARG	Sidechain

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	1585	0	1594	24	0
1	B	1594	0	1597	41	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	44	0	0	1	0
3	B	63	0	0	1	0
All	All	3296	0	3191	63	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 10.

The worst 5 of 63 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:184:GLU:O	1:B:184:GLU:HG2	1.44	1.15
1:B:105:MSE:SE	1:B:147:LEU:HG	2.22	0.88
1:B:182:ARG:O	1:B:183:SER:HB3	1.77	0.85
1:B:182:ARG:O	1:B:183:SER:CB	2.30	0.79
1:A:49:ASN:H	1:A:49:ASN:HD22	1.32	0.77

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	204/235 (87%)	195 (96%)	8 (4%)	1 (0%)	38	45
1	B	204/235 (87%)	191 (94%)	11 (5%)	2 (1%)	22	23
All	All	408/470 (87%)	386 (95%)	19 (5%)	3 (1%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	SER
1	A	87	THR
1	B	140	VAL

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	164/179 (92%)	142 (87%)	22 (13%)	6	5
1	B	165/179 (92%)	148 (90%)	17 (10%)	10	11
All	All	329/358 (92%)	290 (88%)	39 (12%)	8	8

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ARG
1	A	228	GLU
1	B	182	ARG
1	A	167	LYS
1	A	182	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	144	ASN
1	B	41	GLN
1	A	100	GLN
1	B	28	HIS

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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	500	-	4,4,4	0.24	0	6,6,6	0.41	0
2	SO4	B	500	-	4,4,4	0.34	0	6,6,6	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	500	-	-	0/0/0/0	0/0/0/0
2	SO4	B	500	-	-	0/0/0/0	0/0/0/0

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.

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	210/235 (89%)	0.65	26 (12%) 5 7	17, 29, 60, 69	0
1	B	210/235 (89%)	0.60	25 (11%) 5 8	15, 25, 55, 62	0
All	All	420/470 (89%)	0.62	51 (12%) 5 8	15, 27, 58, 69	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	VAL	11.7
1	B	141	GLY	10.4
1	A	185	PHE	9.9
1	A	140	VAL	9.1
1	A	141	GLY	7.3

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

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	500	5/5	0.23	3.10	21,22,22,30	5
2	SO4	A	500	5/5	0.09	-1.59	33,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.