wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 03:37 AM UTC

PDB ID	:	3L6E / pdb_00003l6e
Title	:	Crystal structure of putative short chain dehydrogenase/reductase family oxidoreductase from Aeromonas hydrophila subsp. hydrophila ATCC 7966
Authors	:	Malashkevich, V.N.; Patskovsky, Y.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-12-23
Resolution	:	2.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

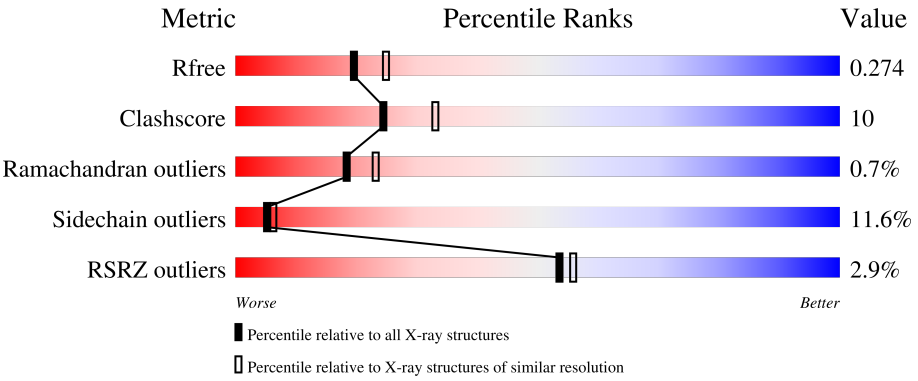
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 <=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	235	2% 70% 17% · 11%
1	B	235	3% 68% 16% 5% 11%

2 Entry composition (i)

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

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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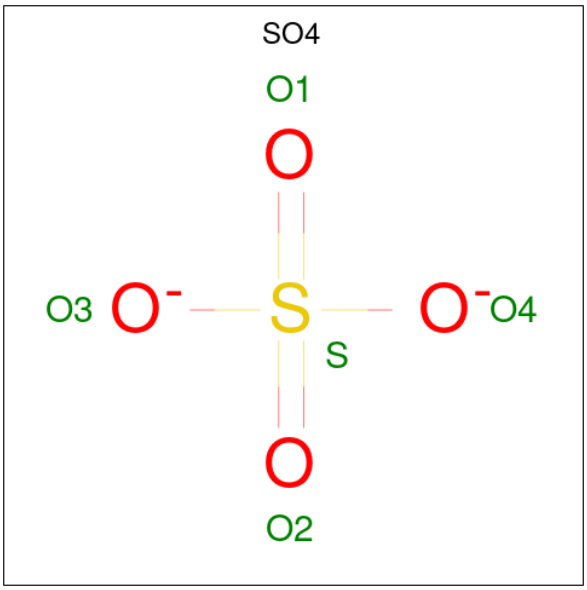
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP A0KPA6
B	3	LEU	-	expression tag	UNP A0KPA6
B	42	GLN	GLU	conflict	UNP A0KPA6
B	45	LEU	GLU	conflict	UNP A0KPA6
B	49	ASN	LYS	conflict	UNP A0KPA6
B	55	VAL	ALA	conflict	UNP A0KPA6
B	63	ASP	GLU	conflict	UNP A0KPA6
B	87	THR	VAL	conflict	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 (CCD ID: SO4) (formula: O_4S).



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

- Molecule 3 is water.

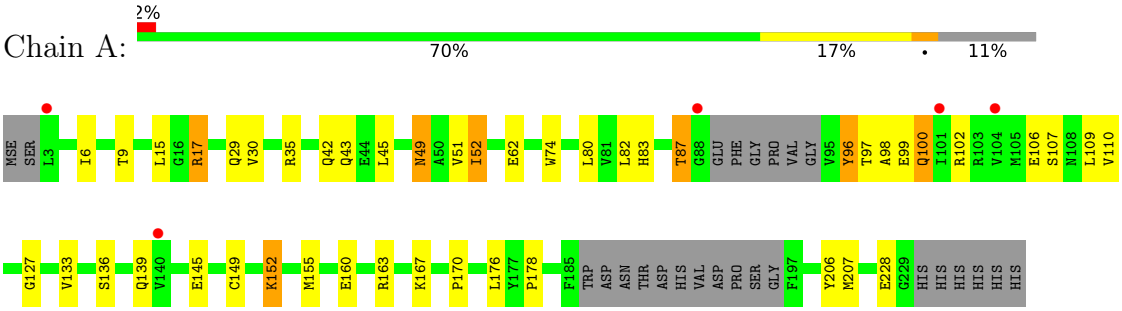
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	44	Total O 44 44	0	0
3	B	63	Total O 63 63	0	0

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.

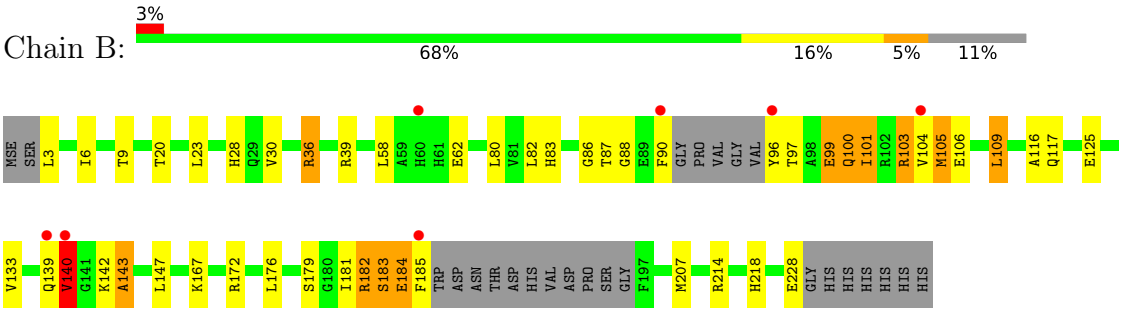
• Molecule 1: Oxidoreductase, short-chain dehydrogenase/reductase family

Chain A:



• Molecule 1: Oxidoreductase, short-chain dehydrogenase/reductase family

Chain B:



4 Data and refinement statistics (i)

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 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.30) 97.5 (20.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.02 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.270 0.228 , 0.274	Depositor DCC
R_{free} test set	1037 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.70	1/1600 (0.1%)	0.92	1/2150 (0.0%)
1	B	0.80	4/1610 (0.2%)	1.02	2/2163 (0.1%)
All	All	0.76	5/3210 (0.2%)	0.97	3/4313 (0.1%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	LEU	C-O	-6.62	1.16	1.24
1	B	116	ALA	C-O	-6.47	1.16	1.24
1	B	116	ALA	CA-CB	-5.72	1.44	1.53
1	B	109	LEU	C-O	-5.56	1.17	1.24
1	B	117	GLN	C-O	-5.00	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	143	ALA	N-CA-C	6.50	118.36	111.28
1	B	86	GLY	N-CA-C	5.76	123.02	115.47
1	A	178	PRO	CB-CA-C	-5.62	107.15	111.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	36	ARG	Sidechain

5.2 Too-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 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	1585	0	1594	25	0
1	B	1594	0	1597	40	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

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 10.

The worst 5 of 63 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:B:184:GLU:HG2	1:B:184:GLU:O	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:HD22	1:A:49:ASN:H	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%)	24 31
1	B	204/235 (87%)	191 (94%)	11 (5%)	2 (1%)	12 15
All	All	408/470 (87%)	386 (95%)	19 (5%)	3 (1%)	18 23

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 (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	164/179 (92%)	144 (88%)	20 (12%)	5 5
1	B	165/179 (92%)	147 (89%)	18 (11%)	6 7
All	All	329/358 (92%)	291 (88%)	38 (12%)	5 6

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	MSE
1	B	182	ARG
1	B	109	LEU
1	B	167	LYS
1	B	228	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN

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Mol	Chain	Res	Type
1	B	28	HIS
1	B	139	GLN
1	B	83	HIS
1	A	83	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 (i)

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	B	500	-	4,4,4	0.25	0	6,6,6	0.43	0
2	SO4	A	500	-	4,4,4	0.21	0	6,6,6	0.45	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.

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

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, 95^{th} 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	204/235 (86%)	0.13	5 (2%)	58	60	17, 29, 60, 69	0
1	B	204/235 (86%)	-0.01	7 (3%)	48	50	15, 25, 55, 62	0
All	All	408/470 (86%)	0.06	12 (2%)	53	56	15, 27, 57, 69	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	VAL	3.6
1	A	101	ILE	3.3
1	A	140	VAL	2.9
1	A	3	LEU	2.8
1	B	185	PHE	2.5

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	SO4	B	500	5/5	0.80	0.15	21,22,22,30	5
2	SO4	A	500	5/5	0.95	0.07	33,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.