



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2024 – 06:00 AM EST

PDB ID : 1T82
Title : Crystal Structure of the putative thioesterase from *Shewanella oneidensis*, Northeast Structural Genomics Target SoR51
Authors : Forouhar, F.; Lee, I.; Vorobiev, S.M.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-05-11
Resolution : 1.70 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

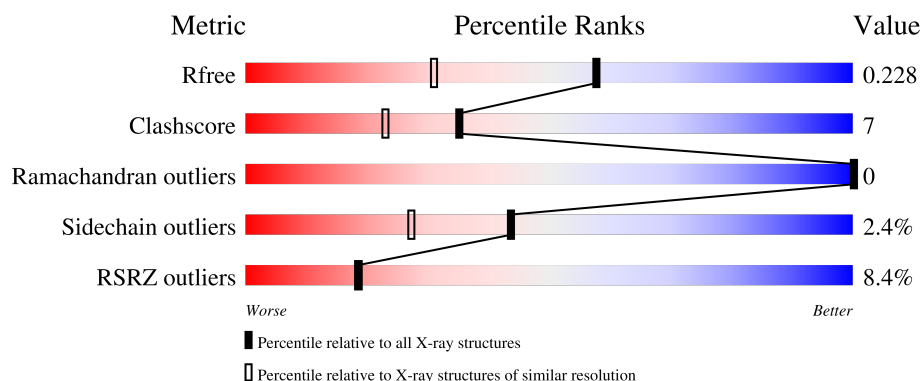
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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 $\leq 5\%$. 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	155	<div> <div>6%</div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
1	B	155	<div> <div>6%</div> <div>74%</div> <div>19%</div> <div>5%</div> </div>
1	C	155	<div> <div>6%</div> <div>79%</div> <div>14%</div> <div>7%</div> </div>
1	D	155	<div> <div>12%</div> <div>70%</div> <div>16%</div> <div>12%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4931 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 hypothetical acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	Se	0	0	0
			1125	724	191	203	2	5			
1	B	147	Total	C	N	O	S	Se	0	0	0
			1165	748	203	207	2	5			
1	C	144	Total	C	N	O	S	Se	0	0	0
			1134	730	193	204	2	5			
1	D	136	Total	C	N	O	S	Se	0	0	0
			1073	692	183	191	2	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MSE	-	expression tag	UNP Q8E989
A	-8	GLY	-	expression tag	UNP Q8E989
A	-7	HIS	-	expression tag	UNP Q8E989
A	-6	HIS	-	expression tag	UNP Q8E989
A	-5	HIS	-	expression tag	UNP Q8E989
A	-4	HIS	-	expression tag	UNP Q8E989
A	-3	HIS	-	expression tag	UNP Q8E989
A	-2	HIS	-	expression tag	UNP Q8E989
A	-1	SER	-	expression tag	UNP Q8E989
A	0	HIS	-	expression tag	UNP Q8E989
A	1	MSE	MET	modified residue	UNP Q8E989
A	22	MSE	MET	modified residue	UNP Q8E989
A	50	MSE	MET	modified residue	UNP Q8E989
A	59	MSE	MET	modified residue	UNP Q8E989
A	66	MSE	MET	modified residue	UNP Q8E989
A	145	MSE	MET	modified residue	UNP Q8E989
B	-10	MSE	-	expression tag	UNP Q8E989
B	-9	GLY	-	expression tag	UNP Q8E989
B	-8	HIS	-	expression tag	UNP Q8E989
B	-7	HIS	-	expression tag	UNP Q8E989
B	-6	HIS	-	expression tag	UNP Q8E989

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8E989
B	-4	HIS	-	expression tag	UNP Q8E989
B	-3	HIS	-	expression tag	UNP Q8E989
B	-3A	SER	-	expression tag	UNP Q8E989
B	-2	HIS	-	expression tag	UNP Q8E989
B	1	MSE	MET	modified residue	UNP Q8E989
B	22	MSE	MET	modified residue	UNP Q8E989
B	50	MSE	MET	modified residue	UNP Q8E989
B	59	MSE	MET	modified residue	UNP Q8E989
B	66	MSE	MET	modified residue	UNP Q8E989
B	145	MSE	MET	modified residue	UNP Q8E989
C	-9	MSE	-	expression tag	UNP Q8E989
C	-8	GLY	-	expression tag	UNP Q8E989
C	-7	HIS	-	expression tag	UNP Q8E989
C	-6	HIS	-	expression tag	UNP Q8E989
C	-5	HIS	-	expression tag	UNP Q8E989
C	-4	HIS	-	expression tag	UNP Q8E989
C	-3	HIS	-	expression tag	UNP Q8E989
C	-2	HIS	-	expression tag	UNP Q8E989
C	-1	SER	-	expression tag	UNP Q8E989
C	0	HIS	-	expression tag	UNP Q8E989
C	1	MSE	MET	modified residue	UNP Q8E989
C	22	MSE	MET	modified residue	UNP Q8E989
C	50	MSE	MET	modified residue	UNP Q8E989
C	59	MSE	MET	modified residue	UNP Q8E989
C	66	MSE	MET	modified residue	UNP Q8E989
C	145	MSE	MET	modified residue	UNP Q8E989
D	-9	MSE	-	expression tag	UNP Q8E989
D	-8	GLY	-	expression tag	UNP Q8E989
D	-7	HIS	-	expression tag	UNP Q8E989
D	-6	HIS	-	expression tag	UNP Q8E989
D	-5	HIS	-	expression tag	UNP Q8E989
D	-4	HIS	-	expression tag	UNP Q8E989
D	-3	HIS	-	expression tag	UNP Q8E989
D	-2	HIS	-	expression tag	UNP Q8E989
D	-1	SER	-	expression tag	UNP Q8E989
D	0	HIS	-	expression tag	UNP Q8E989
D	1	MSE	MET	modified residue	UNP Q8E989
D	22	MSE	MET	modified residue	UNP Q8E989
D	50	MSE	MET	modified residue	UNP Q8E989
D	59	MSE	MET	modified residue	UNP Q8E989
D	66	MSE	MET	modified residue	UNP Q8E989

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Chain	Residue	Modelled	Actual	Comment	Reference
D	145	MSE	MET	modified residue	UNP Q8E989

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total 84	O 84	0	0
2	B	112	Total 112	O 112	0	0
2	C	128	Total 128	O 128	0	0
2	D	110	Total 110	O 110	0	0

- Molecule 1: hypothetical acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.98Å 49.67Å 99.67Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	29.81 – 1.70 29.81 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.9 (29.81-1.70) 96.6 (29.81-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.34 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.222 0.202 , 0.228	Depositor DCC
R_{free} test set	5626 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4931	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.56% 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	0.31	0/1149	0.55	0/1561
1	B	0.29	0/1192	0.54	0/1618
1	C	0.29	0/1157	0.54	0/1569
1	D	0.30	0/1095	0.54	0/1484
All	All	0.30	0/4593	0.54	0/6232

There are no bond length outliers.

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	1125	0	1135	9	0
1	B	1165	0	1165	20	0
1	C	1134	0	1145	12	0
1	D	1073	0	1083	25	0
2	A	84	0	0	1	0
2	B	112	0	0	3	0
2	C	128	0	0	1	0
2	D	110	0	0	1	0
All	All	4931	0	4528	66	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 7.

The worst 5 of 66 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:118:LYS:HG2	1:A:140:VAL:HG22	1.72	0.71
1:A:88:ARG:HH21	1:A:134:GLN:HG2	1.55	0.71
1:D:66:MSE:HE2	1:D:70:GLN:HG2	1.77	0.67
1:B:-5:HIS:HB2	1:B:6:ASN:HD21	1.59	0.66
1:D:45:ASN:C	1:D:45:ASN:HD22	1.98	0.64

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	141/155 (91%)	139 (99%)	2 (1%)	0	100	100
1	B	143/155 (92%)	140 (98%)	3 (2%)	0	100	100
1	C	142/155 (92%)	138 (97%)	4 (3%)	0	100	100
1	D	132/155 (85%)	128 (97%)	4 (3%)	0	100	100
All	All	558/620 (90%)	545 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	125/129 (97%)	123 (98%)	2 (2%)	58	44
1	B	129/129 (100%)	123 (95%)	6 (5%)	22	8
1	C	126/129 (98%)	125 (99%)	1 (1%)	79	71
1	D	118/129 (92%)	115 (98%)	3 (2%)	42	25
All	All	498/516 (96%)	486 (98%)	12 (2%)	44	27

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	116	LYS
1	C	136	ASP
1	D	113	ARG
1	D	45	ASN
1	B	31	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	GLN
1	D	6	ASN
1	B	134	GLN
1	D	45	ASN
1	C	71	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	-2:HIS	C	1:MSE	N	6.94

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	138/155 (89%)	0.25	10 (7%) 23 23	4, 11, 26, 32	0
1	B	142/155 (91%)	0.29	9 (6%) 27 28	5, 12, 24, 30	0
1	C	139/155 (89%)	0.29	9 (6%) 26 27	5, 14, 24, 30	0
1	D	131/155 (84%)	0.59	18 (13%) 8 7	5, 14, 28, 31	0
All	All	550/620 (88%)	0.35	46 (8%) 18 18	4, 13, 26, 32	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-2	HIS	5.5
1	D	113	ARG	4.8
1	C	136	ASP	4.0
1	D	76	VAL	4.0
1	D	114	GLY	3.9

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 monosaccharides 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.