



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:03 PM GMT

PDB ID : 4FGI
Title : Structure of the effector - immunity system Tse1 / Tsi1 from *Pseudomonas aeruginosa*
Authors : Benz, J.; Sendlmeier, C.; Barends, T.R.M.; Meinhart, A.
Deposited on : 2012-06-04
Resolution : 3.20 Å(reported)

This is a full wwPDB validation 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>

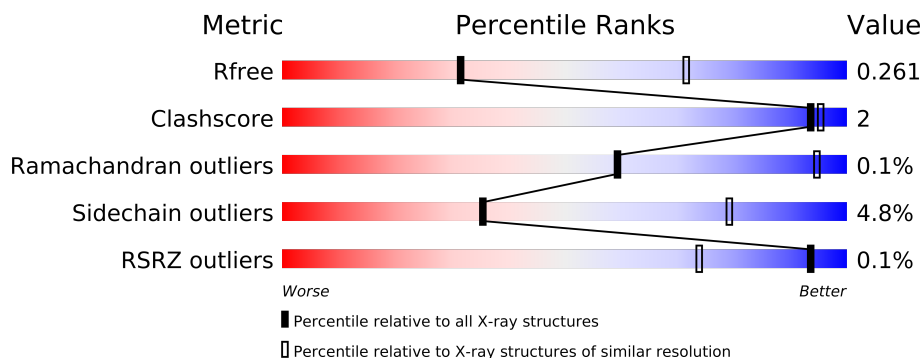
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	165	
1	C	165	
1	E	165	
1	G	165	
2	B	151	
2	D	151	
2	F	151	
2	H	151	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8893 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 Tse1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	Se	0	0	0
			1097	685	196	207	6	3			
1	C	146	Total	C	N	O	S	Se	0	0	0
			1091	682	195	205	6	3			
1	E	146	Total	C	N	O	S	Se	0	0	0
			1091	682	195	205	6	3			
1	G	145	Total	C	N	O	S	Se	0	0	0
			1085	679	194	203	6	3			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
A	156	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
A	157	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
A	158	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
A	159	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
A	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	163	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	164	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	165	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	155	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
C	156	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
C	157	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
C	158	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
C	159	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
C	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	163	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	164	HIS	-	EXPRESSION TAG	UNP Q9I2Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	165	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	155	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
E	156	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
E	157	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
E	158	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
E	159	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
E	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	163	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	164	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	165	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	155	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
G	156	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
G	157	ALA	-	EXPRESSION TAG	UNP Q9I2Q1
G	158	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
G	159	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
G	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	163	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	164	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	165	HIS	-	EXPRESSION TAG	UNP Q9I2Q1

- Molecule 2 is a protein called Tsi1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	147	Total	C	N	O	S	Se	0	0	0
			1134	697	201	228	5	3			
2	D	147	Total	C	N	O	S	Se	0	0	0
			1134	697	201	228	5	3			
2	F	147	Total	C	N	O	S	Se	0	0	0
			1134	697	201	228	5	3			
2	H	146	Total	C	N	O	S	Se	0	0	0
			1127	693	200	226	5	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	MSE	-	EXPRESSION TAG	UNP Q9I2Q0
B	23	ALA	-	EXPRESSION TAG	UNP Q9I2Q0
D	22	MSE	-	EXPRESSION TAG	UNP Q9I2Q0

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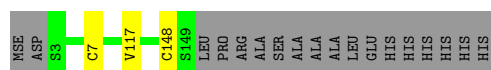
Chain	Residue	Modelled	Actual	Comment	Reference
D	23	ALA	-	EXPRESSION TAG	UNP Q9I2Q0
F	22	MSE	-	EXPRESSION TAG	UNP Q9I2Q0
F	23	ALA	-	EXPRESSION TAG	UNP Q9I2Q0
H	22	MSE	-	EXPRESSION TAG	UNP Q9I2Q0
H	23	ALA	-	EXPRESSION TAG	UNP Q9I2Q0

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.

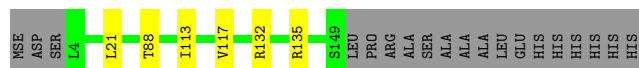
- Molecule 1: Tse1

Chain A: 



- Molecule 1: Tse1

Chain C: 



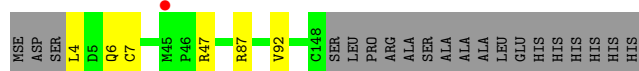
- Molecule 1: Tse1

Chain E: 



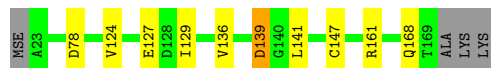
- Molecule 1: Tse1

Chain G: 



- Molecule 2: Tsi1

Chain B: 



- Molecule 2: Tsi1

Chain D: 



- Molecule 2: Tsi1

Chain F: 



● Molecule 2: Tsi1

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.56Å 97.56Å 423.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 3.20 49.35 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.33-3.20) 99.9 (49.35-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.263 0.222 , 0.261	Depositor DCC
R_{free} test set	1753 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 15.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35044 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8893	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.32	0/1116	0.47	0/1507
1	C	0.32	0/1110	0.48	0/1499
1	E	0.33	0/1110	0.48	0/1499
1	G	0.32	0/1104	0.48	0/1491
2	B	0.37	0/1155	0.55	0/1555
2	D	0.37	0/1155	0.51	0/1555
2	F	0.34	0/1155	0.51	0/1555
2	H	0.37	0/1148	0.55	0/1545
All	All	0.35	0/9053	0.50	0/12206

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1097	0	0	0	0
1	C	1091	0	0	1	0
1	E	1091	0	0	1	0
1	G	1085	0	0	0	0
2	B	1134	0	0	4	0
2	D	1134	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1134	0	0	3	0
2	H	1127	0	0	4	0
All	All	8893	0	0	14	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 2.

All (14) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:23:ALA:N	2:D:167:CYS:SG	2.75	0.60
2:F:100:ARG:NH1	2:F:168:GLN:OE1	2.42	0.52
2:B:127:GLU:OE2	2:B:161:ARG:NE	2.43	0.51
2:F:23:ALA:N	2:F:167:CYS:SG	2.89	0.46
2:B:168:GLN:NE2	2:D:126:ARG:O	2.50	0.45
2:F:42:GLU:OE1	2:F:47:ARG:NH1	2.50	0.45
1:C:135:ARG:NH1	2:D:65:GLU:OE2	2.50	0.44
2:B:129:ILE:CG2	2:B:129:ILE:O	2.66	0.44
2:H:139:ASP:N	2:H:139:ASP:OD1	2.50	0.44
2:B:139:ASP:OD1	2:B:139:ASP:N	2.51	0.43
2:H:133:ARG:NE	2:H:149:GLY:O	2.52	0.43
1:E:6:GLN:O	1:E:10:ASN:N	2.52	0.43
2:H:105:GLU:OE2	2:H:116:TYR:OH	2.37	0.42
2:H:127:GLU:OE2	2:H:161:ARG:NE	2.52	0.42

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	145/165 (88%)	141 (97%)	4 (3%)	0	100	100
1	C	144/165 (87%)	136 (94%)	8 (6%)	0	100	100
1	E	144/165 (87%)	137 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	143/165 (87%)	137 (96%)	6 (4%)	0	100	100
2	B	145/151 (96%)	140 (97%)	5 (3%)	0	100	100
2	D	145/151 (96%)	139 (96%)	5 (3%)	1 (1%)	30	80
2	F	145/151 (96%)	138 (95%)	7 (5%)	0	100	100
2	H	144/151 (95%)	138 (96%)	6 (4%)	0	100	100
All	All	1155/1264 (91%)	1106 (96%)	48 (4%)	1 (0%)	59	95

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	168	GLN

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	114/124 (92%)	111 (97%)	3 (3%)	59	90
1	C	113/124 (91%)	108 (96%)	5 (4%)	39	81
1	E	113/124 (91%)	104 (92%)	9 (8%)	17	57
1	G	112/124 (90%)	106 (95%)	6 (5%)	31	75
2	B	125/124 (101%)	119 (95%)	6 (5%)	35	79
2	D	125/124 (101%)	123 (98%)	2 (2%)	75	94
2	F	125/124 (101%)	117 (94%)	8 (6%)	25	69
2	H	124/124 (100%)	117 (94%)	7 (6%)	30	75
All	All	951/992 (96%)	905 (95%)	46 (5%)	35	79

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	CYS
1	A	117	VAL
1	A	148	CYS

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Mol	Chain	Res	Type
2	B	78	ASP
2	B	124	VAL
2	B	136	VAL
2	B	139	ASP
2	B	141	LEU
2	B	147	CYS
1	C	21	LEU
1	C	88	THR
1	C	113	ILE
1	C	117	VAL
1	C	132	ARG
2	D	147	CYS
2	D	169	THR
1	E	4	LEU
1	E	7	CYS
1	E	21	LEU
1	E	47	ARG
1	E	55	ASP
1	E	66	SER
1	E	88	THR
1	E	132	ARG
1	E	148	CYS
2	F	27	LEU
2	F	49	MSE
2	F	65	GLU
2	F	70	LEU
2	F	122	LYS
2	F	139	ASP
2	F	147	CYS
2	F	150	GLU
1	G	4	LEU
1	G	6	GLN
1	G	7	CYS
1	G	47	ARG
1	G	87	ARG
1	G	92	VAL
2	H	25	THR
2	H	96	GLN
2	H	99	ARG
2	H	110	SER
2	H	129	ILE
2	H	139	ASP

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Mol	Chain	Res	Type
2	H	147	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no ligands in this entry.

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	147/165 (89%)	-0.06	0	100	100	46, 73, 102, 117	1 (0%)
1	C	146/165 (88%)	-0.19	0	100	100	41, 67, 95, 123	1 (0%)
1	E	146/165 (88%)	-0.07	0	100	100	53, 90, 132, 157	1 (0%)
1	G	145/165 (87%)	0.06	1 (0%)	84	38	53, 84, 122, 130	1 (0%)
2	B	147/151 (97%)	-0.12	0	100	100	40, 56, 81, 91	0
2	D	147/151 (97%)	-0.08	0	100	100	37, 57, 87, 99	0
2	F	147/151 (97%)	-0.08	0	100	100	42, 65, 106, 127	0
2	H	146/151 (96%)	-0.01	0	100	100	48, 76, 104, 117	0
All	All	1171/1264 (92%)	-0.07	1 (0%)	93	74	37, 70, 115, 157	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	45	MSE	3.0

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.