



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:45 PM GMT

PDB ID : 4HTT  
Title : Crystal Structure of Twin Arginine Translocase Receptor- TatC in DDM  
Authors : Ramasamy, S.; Suloway, C.J.M.; Clemons Jr., W.M.  
Deposited on : 2012-11-01  
Resolution : 6.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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

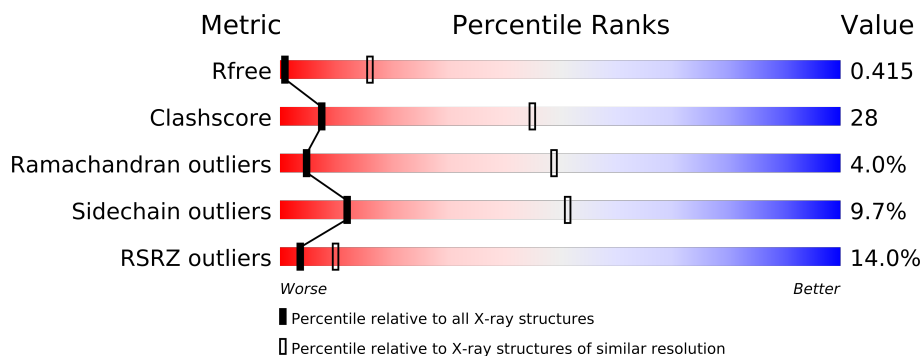
MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683



# 1 Overall quality at a glance



The reported resolution of this entry is 6.80 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	1098 (10.00-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RSRZ outliers	66119	1097 (10.00-3.50)

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  $\geq 3$ , 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	418	
1	B	418	



## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3608 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 Sec-independent protein translocase protein TatC, Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	16	0	0
			1804	1248	263	289	4			
1	B	225	Total	C	N	O	S	16	0	0
			1804	1248	263	289	4			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP O67305
A	0	GLY	-	EXPRESSION TAG	UNP O67305
A	236	GLU	-	EXPRESSION TAG	UNP P00720
A	237	ILE	-	EXPRESSION TAG	UNP P00720
A	238	GLY	-	EXPRESSION TAG	UNP P00720
A	239	SER	-	EXPRESSION TAG	UNP P00720
A	240	GLY	-	EXPRESSION TAG	UNP P00720
A	241	ALA	-	EXPRESSION TAG	UNP P00720
A	242	SER	-	EXPRESSION TAG	UNP P00720
A	296	THR	CYS	CONFLICT	UNP P00720
A	339	ALA	CYS	CONFLICT	UNP P00720
A	407	GLU	-	EXPRESSION TAG	UNP P00720
A	408	LEU	-	EXPRESSION TAG	UNP P00720
A	409	TYR	-	EXPRESSION TAG	UNP P00720
A	410	LYS	-	EXPRESSION TAG	UNP P00720
A	411	HIS	-	EXPRESSION TAG	UNP P00720
A	412	HIS	-	EXPRESSION TAG	UNP P00720
A	413	HIS	-	EXPRESSION TAG	UNP P00720
A	414	HIS	-	EXPRESSION TAG	UNP P00720
B	-1	MET	-	EXPRESSION TAG	UNP O67305
B	0	GLY	-	EXPRESSION TAG	UNP O67305
B	236	GLU	-	EXPRESSION TAG	UNP P00720
B	237	ILE	-	EXPRESSION TAG	UNP P00720
B	238	GLY	-	EXPRESSION TAG	UNP P00720
B	239	SER	-	EXPRESSION TAG	UNP P00720

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Chain	Residue	Modelled	Actual	Comment	Reference
B	240	GLY	-	EXPRESSION TAG	UNP P00720
B	241	ALA	-	EXPRESSION TAG	UNP P00720
B	242	SER	-	EXPRESSION TAG	UNP P00720
B	296	THR	CYS	CONFLICT	UNP P00720
B	339	ALA	CYS	CONFLICT	UNP P00720
B	407	GLU	-	EXPRESSION TAG	UNP P00720
B	408	LEU	-	EXPRESSION TAG	UNP P00720
B	409	TYR	-	EXPRESSION TAG	UNP P00720
B	410	LYS	-	EXPRESSION TAG	UNP P00720
B	411	HIS	-	EXPRESSION TAG	UNP P00720
B	412	HIS	-	EXPRESSION TAG	UNP P00720
B	413	HIS	-	EXPRESSION TAG	UNP P00720
B	414	HIS	-	EXPRESSION TAG	UNP P00720

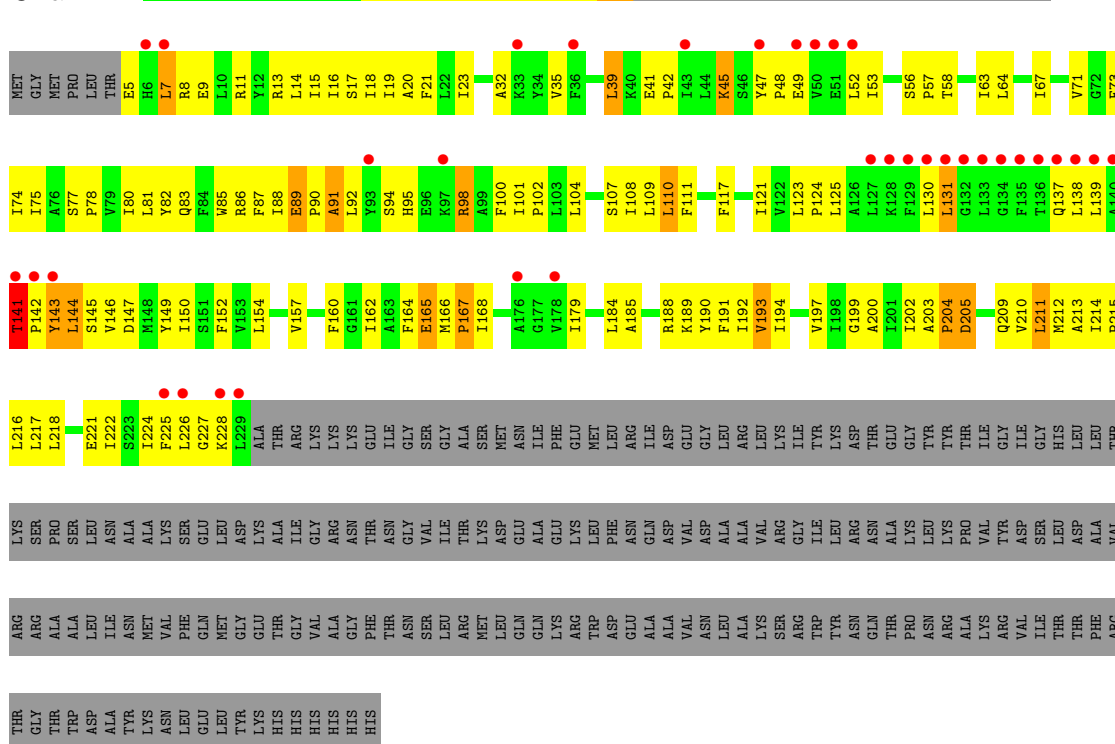


### 3 Residue-property plots

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: Sec-independent protein translocase protein TatC, Lysozyme

Chain A:

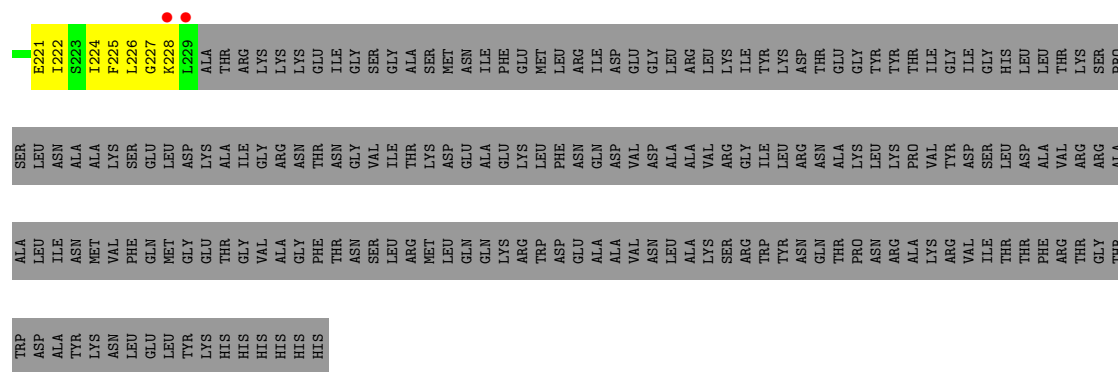


- Molecule 1: Sec-independent protein translocase protein TatC, Lysozyme

Chain B:









## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.01Å 142.01Å 251.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 6.80 39.25 – 6.80	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-6.80) 95.0 (39.25-6.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 6.64Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.344 , 0.418 0.348 , 0.415	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	409.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 694.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 2281 reflections	Xtriage
$F_o, F_c$ correlation	0.70	EDS
Total number of atoms	3608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	474.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.28	0/1853	0.49	0/2522
1	B	0.28	0/1853	0.49	0/2522
All	All	0.28	0/3706	0.49	0/5044

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	1804	0	1946	104	0
1	B	1804	0	1946	108	2
All	All	3608	0	3892	207	2

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 28.

The worst 5 of 207 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:LYS:HB3	1:B:206:VAL:HG22	1.48	0.96
1:A:214:ILE:HA	1:A:217:LEU:HD12	1.54	0.89
1:A:141:THR:HG23	1:A:142:PRO:HD2	1.56	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:141:THR:HG23	1:B:142:PRO:HD2	1.59	0.85
1:A:164:PHE:O	1:A:167:PRO:HD2	1.80	0.81

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:95:HIS:NE2	1:B:95:HIS:NE2[8_775]	1.93	0.27
1:B:22:LEU:CD1	1:B:22:LEU:CD1[6_565]	2.13	0.07

## 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	223/418 (53%)	192 (86%)	22 (10%)	9 (4%)	5	49
1	B	223/418 (53%)	193 (86%)	21 (9%)	9 (4%)	5	49
All	All	446/836 (53%)	385 (86%)	43 (10%)	18 (4%)	5	49

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	141	THR
1	A	211	LEU
1	B	94	SER
1	B	141	THR

### 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	195/356 (55%)	176 (90%)	19 (10%)	12	51
1	B	195/356 (55%)	176 (90%)	19 (10%)	12	51
All	All	390/712 (55%)	352 (90%)	38 (10%)	12	51

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

Mol	Chain	Res	Type
1	A	193	VAL
1	B	39	LEU
1	B	165	GLU
1	B	7	LEU
1	B	45	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	B	137	GLN
1	B	209	GLN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	225/418 (53%)	0.86	35 (15%) 3 9	212, 472, 626, 717	4 (1%)
1	B	225/418 (53%)	0.63	28 (12%) 5 12	211, 472, 626, 717	4 (1%)
All	All	450/836 (53%)	0.75	63 (14%) 3 10	211, 472, 638, 717	8 (1%)

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	THR	10.1
1	A	134	GLY	9.8
1	A	133	LEU	7.6
1	A	137	GLN	7.5
1	A	135	PHE	7.0

### 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.