



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:31 am BST

PDB ID : 6EBA  
Title : Crystal Structure of A Bacterial Homolog to Human Lysosomal Transporter, Spinster, in Inward-facing And Unoccupied Conformation  
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Deposited on : 2018-08-06  
Resolution : 3.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

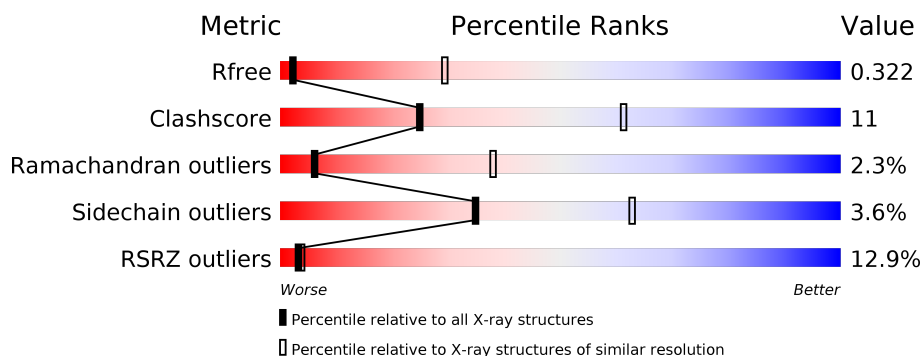
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.81 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))
$R_{free}$	130704	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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 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	508	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3628 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 Major facilitator family transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3628	2412	582	614	20			

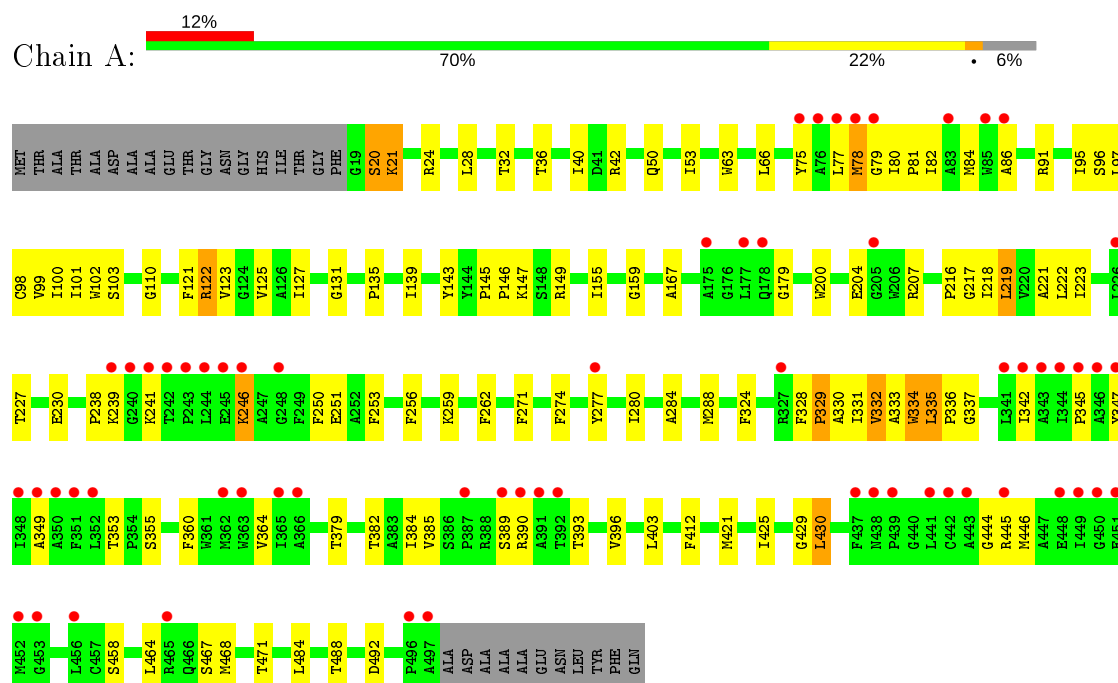
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	ALA	-	expression tag	UNP Q0C3L7
A	501	ALA	-	expression tag	UNP Q0C3L7
A	502	ALA	-	expression tag	UNP Q0C3L7
A	503	GLU	-	expression tag	UNP Q0C3L7
A	504	ASN	-	expression tag	UNP Q0C3L7
A	505	LEU	-	expression tag	UNP Q0C3L7
A	506	TYR	-	expression tag	UNP Q0C3L7
A	507	PHE	-	expression tag	UNP Q0C3L7
A	508	GLN	-	expression tag	UNP Q0C3L7

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Major facilitator family transporter



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.63Å 98.49Å 125.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.81 49.24 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.24-3.81) 84.4 (49.24-3.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.315 , 0.326 0.315 , 0.322	Depositor DCC
$R_{free}$ test set	1107 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	144.1	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 114.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	3628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.27	0/3735	0.45	0/5095

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	3628	0	3688	79	0
All	All	3628	0	3688	79	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 11.

All (79) 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:100:ILE:HG13	1:A:218:ILE:HD12	1.59	0.84
1:A:332:VAL:HG21	1:A:337:GLY:HA2	1.63	0.81
1:A:20:SER:O	1:A:24:ARG:NH1	2.22	0.72
1:A:86:ALA:O	1:A:91:ARG:NH2	2.23	0.70
1:A:467:SER:O	1:A:471:THR:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:VAL:HG11	1:A:393:THR:HG21	1.77	0.67
1:A:421:MET:O	1:A:425:ILE:HG12	1.95	0.66
1:A:99:VAL:HB	1:A:221:ALA:HB2	1.77	0.66
1:A:349:ALA:O	1:A:353:THR:OG1	2.14	0.66
1:A:379:THR:O	1:A:382:THR:HG22	1.97	0.64
1:A:146:PRO:HA	1:A:149:ARG:HG3	1.79	0.64
1:A:95:ILE:HD11	1:A:135:PRO:HB2	1.79	0.63
1:A:464:LEU:O	1:A:468:MET:HG2	1.99	0.62
1:A:78:MET:O	1:A:82:ILE:HG13	2.01	0.60
1:A:100:ILE:HG22	1:A:101:ILE:HD12	1.84	0.59
1:A:259:LYS:NZ	1:A:384:ILE:O	2.32	0.58
1:A:204:GLU:N	1:A:204:GLU:OE1	2.36	0.56
1:A:42:ARG:O	1:A:122:ARG:NH2	2.39	0.55
1:A:484:LEU:O	1:A:488:THR:HG22	2.06	0.55
1:A:77:LEU:O	1:A:79:GLY:N	2.39	0.55
1:A:425:ILE:HG23	1:A:430:LEU:HD12	1.89	0.54
1:A:412:PHE:CD1	1:A:471:THR:HG22	2.43	0.54
1:A:20:SER:OG	1:A:21:LYS:N	2.40	0.53
1:A:425:ILE:O	1:A:429:GLY:N	2.40	0.53
1:A:219:LEU:HA	1:A:222:LEU:HD12	1.90	0.53
1:A:444:GLY:O	1:A:446:MET:N	2.41	0.53
1:A:334:TRP:CE3	1:A:335:LEU:HG	2.45	0.52
1:A:382:THR:O	1:A:390:ARG:NH2	2.38	0.51
1:A:32:THR:HG21	1:A:155:ILE:HD12	1.91	0.51
1:A:335:LEU:H	1:A:336:PRO:HD2	1.75	0.51
1:A:91:ARG:O	1:A:95:ILE:HD12	2.11	0.51
1:A:145:PRO:HB2	1:A:147:LYS:HD2	1.93	0.51
1:A:147:LYS:HD2	1:A:147:LYS:H	1.76	0.50
1:A:82:ILE:HD13	1:A:131:GLY:HA2	1.92	0.50
1:A:91:ARG:HB2	1:A:139:ILE:HD11	1.94	0.50
1:A:223:ILE:O	1:A:227:THR:OG1	2.26	0.50
1:A:84:MET:N	1:A:84:MET:SD	2.85	0.49
1:A:253:PHE:HA	1:A:256:PHE:CE2	2.47	0.49
1:A:353:THR:HG22	1:A:355:SER:H	1.77	0.49
1:A:28:LEU:O	1:A:32:THR:HG23	2.13	0.48
1:A:412:PHE:HD1	1:A:471:THR:HG22	1.77	0.48
1:A:342:ILE:O	1:A:345:PRO:HD2	2.14	0.47
1:A:40:ILE:HA	1:A:167:ALA:HB2	1.95	0.47
1:A:335:LEU:H	1:A:336:PRO:CD	2.28	0.47
1:A:179:GLY:O	1:A:200:TRP:HB3	2.15	0.47
1:A:103:SER:OG	1:A:217:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:O	1:A:125:VAL:HG23	2.14	0.46
1:A:251:GLU:N	1:A:251:GLU:OE2	2.49	0.46
1:A:218:ILE:HG23	1:A:219:LEU:N	2.31	0.46
1:A:250:PHE:O	1:A:253:PHE:HB3	2.16	0.46
1:A:332:VAL:HG22	1:A:333:ALA:H	1.79	0.46
1:A:100:ILE:HG13	1:A:218:ILE:CD1	2.40	0.44
1:A:91:ARG:HG2	1:A:91:ARG:H	1.64	0.44
1:A:219:LEU:O	1:A:223:ILE:HG22	2.18	0.44
1:A:36:THR:HG22	1:A:159:GLY:HA2	1.99	0.44
1:A:123:VAL:O	1:A:127:ILE:HG12	2.17	0.43
1:A:389:SER:O	1:A:393:THR:HG23	2.18	0.43
1:A:284:ALA:O	1:A:288:MET:HG2	2.18	0.43
1:A:329:PRO:O	1:A:331:ILE:N	2.52	0.43
1:A:360:PHE:O	1:A:364:VAL:HG13	2.19	0.43
1:A:216:PRO:HA	1:A:219:LEU:HD21	2.01	0.43
1:A:262:PHE:HZ	1:A:396:VAL:HG23	1.84	0.42
1:A:271:PHE:HA	1:A:274:PHE:HB3	2.01	0.42
1:A:50:GLN:NE2	1:A:53:ILE:HD11	2.35	0.42
1:A:96:SER:HA	1:A:221:ALA:HB1	2.02	0.42
1:A:97:LEU:O	1:A:101:ILE:HD13	2.19	0.42
1:A:110:GLY:O	1:A:207:ARG:NH2	2.44	0.42
1:A:21:LYS:HD3	1:A:24:ARG:HH12	1.84	0.42
1:A:80:ILE:HB	1:A:81:PRO:HD3	2.01	0.42
1:A:99:VAL:HG22	1:A:102:TRP:CZ2	2.54	0.42
1:A:28:LEU:HG	1:A:155:ILE:HD11	2.02	0.42
1:A:384:ILE:HD11	1:A:492:ASP:HB3	2.02	0.41
1:A:277:TYR:HA	1:A:280:ILE:HG22	2.02	0.41
1:A:146:PRO:HG3	1:A:149:ARG:NH1	2.36	0.41
1:A:256:PHE:HB3	1:A:385:VAL:HG21	2.02	0.41
1:A:63:TRP:CZ3	1:A:66:LEU:HD23	2.56	0.40
1:A:98:CYS:O	1:A:102:TRP:CD1	2.75	0.40
1:A:95:ILE:O	1:A:99:VAL:HG23	2.21	0.40
1:A:403:LEU:HD23	1:A:403:LEU:HA	1.88	0.40

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	477/508 (94%)	430 (90%)	36 (8%)	11 (2%)	6	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ALA
1	A	445	ARG
1	A	78	MET
1	A	332	VAL
1	A	20	SER
1	A	21	LYS
1	A	238	PRO
1	A	246	LYS
1	A	324	PHE
1	A	329	PRO
1	A	335	LEU

### 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	366/384 (95%)	353 (96%)	13 (4%)	35	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	TYR
1	A	122	ARG
1	A	143	TYR
1	A	219	LEU
1	A	230	GLU
1	A	239	LYS
1	A	241	LYS
1	A	246	LYS
1	A	328	PHE
1	A	334	TRP
1	A	347	TYR
1	A	430	LEU
1	A	458	SER

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

### 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 carbohydrates 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](#)

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	479/508 (94%)	0.44	62 (12%) 3 4	143, 184, 241, 282	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	ILE	9.6
1	A	441	LEU	9.3
1	A	243	PRO	6.3
1	A	452	MET	5.7
1	A	241	LYS	5.6
1	A	352	LEU	5.6
1	A	351	PHE	5.1
1	A	327	ARG	5.1
1	A	245	GLU	4.8
1	A	79	GLY	4.8
1	A	450	GLY	4.7
1	A	347	TYR	4.7
1	A	244	LEU	4.7
1	A	242	THR	4.6
1	A	76	ALA	4.6
1	A	246	LYS	4.6
1	A	453	GLY	4.5
1	A	496	PRO	4.4
1	A	443	ALA	4.2
1	A	343	ALA	4.2
1	A	392	THR	4.1
1	A	177	LEU	3.9
1	A	390	ARG	3.7
1	A	348	ILE	3.7
1	A	78	MET	3.6
1	A	345	PRO	3.5
1	A	438	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	442	CYS	3.3
1	A	349	ALA	3.2
1	A	346	ALA	3.2
1	A	387	PRO	3.2
1	A	365	ILE	3.2
1	A	178	GLN	3.1
1	A	341	LEU	3.1
1	A	448	GLU	3.1
1	A	85	TRP	3.1
1	A	240	GLY	3.0
1	A	437	PHE	3.0
1	A	342	ILE	2.9
1	A	77	LEU	2.8
1	A	391	ALA	2.8
1	A	445	ARG	2.8
1	A	456	LEU	2.8
1	A	175	ALA	2.7
1	A	277	TYR	2.7
1	A	350	ALA	2.7
1	A	465	ARG	2.6
1	A	363	TRP	2.5
1	A	366	ALA	2.5
1	A	248	GLY	2.3
1	A	451	GLU	2.3
1	A	83	ALA	2.3
1	A	226	LEU	2.3
1	A	239	LYS	2.2
1	A	86	ALA	2.2
1	A	205	GLY	2.2
1	A	344	ILE	2.1
1	A	362	MET	2.1
1	A	75	TYR	2.1
1	A	439	PRO	2.1
1	A	497	ALA	2.0
1	A	389	SER	2.0

## 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 [i](#)

There are no carbohydrates 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.