



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:21 PM GMT

PDB ID : 4LDS
Title : The inward-facing structure of the glucose transporter from *Staphylococcus epidermidis*
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Deposited on : 2013-06-25
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

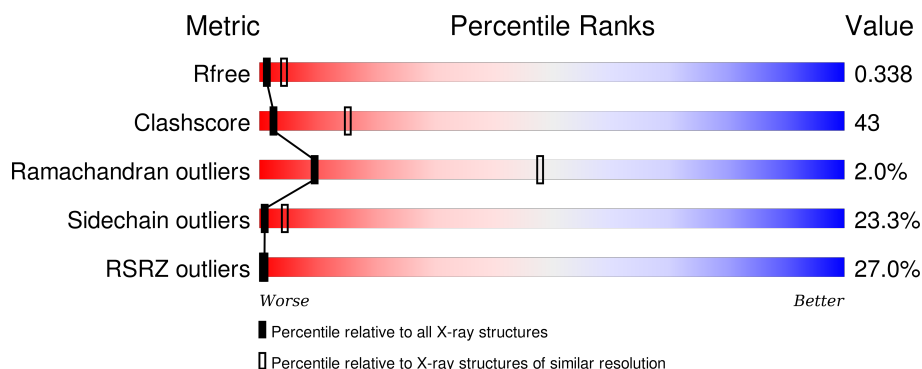
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	446	
1	B	446	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6388 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.

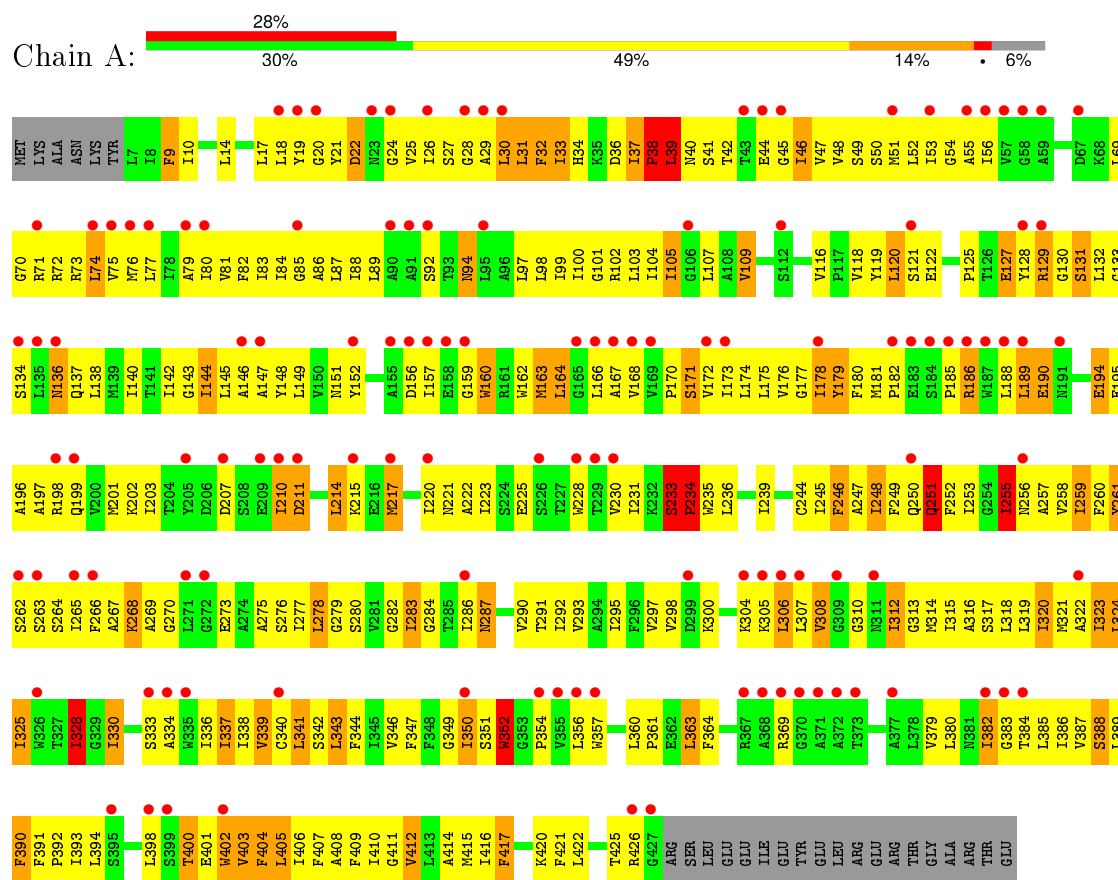
- Molecule 1 is a protein called Bicyclomycin resistance protein TcaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3194	2127	503	548	16			
1	B	421	Total	C	N	O	S	0	0	0
			3194	2127	503	548	16			

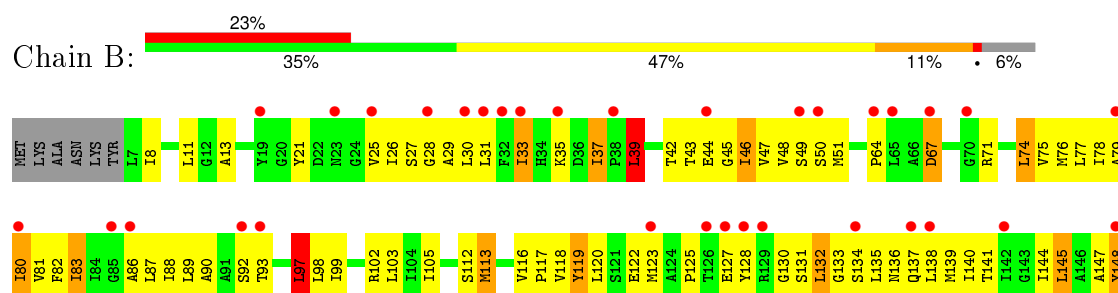
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: Bicyclomycin resistance protein TcaB



• Molecule 1: Bicyclomycin resistance protein TcaB



L405	L406	F407	A408	F409	I410	O411	V412	L413	A414	N415	I416	F417	V418	I419	F420	F421	L422	P423	E424	T425	R426	G427	ARG	SER	LEU	GLU	GLU	ILE	GLU	TVR	GLU	LEU	ARG	GLU	ARG	ALA	ARG	THR	GLU																		
C340	L341	S342	I345	V346	F347	F348	G349	I350	S351	N352	G353	P354	V355	L356	W357	V358	N359	L360	P361	E362	L363	R367	A368	R369	G370	A371	A372	T373	G374	I375	S376	A377	L378	V379	L380	N381	I382	G383	V387	S388	L389	F390	F391	P392	I393	L394	S395	D396	A397	L398	S399	T400	E401	W402	V403	F404	
L278	G279	S280	V281	I283	G284	T285	L286	N287	V288	L289	V290	T291	L292	V293	F296	V297	V298	D299	K300	I301	D302	R303	K304	K305	L306	A307	V308	G309	G310	N311	I312	G313	M314	I315	A316	S317	L318	L319	I320	M321	A322	I323	L324	I325	W326	T327	I328	A331	S332	S333	A334	W335	I336	I337	V339		
D211	K212	E213	L214	M217	K218	E219	I220	T227	W228	T229	V230	I231	K232	S233	P234	W235	L236	G237	R238	I239	L240	I241	V242	G243	C244	I245	F246	A247	I248	F249	Q250	Q251	F252	I253	G254	I255	W256	A257	V258	I259	F260	Y261	S262	S263	W264	I265	F266	A267	K268	A269	G270	E273	A274	A275	S276	I277	
N151	Y152	A153	F154	A155	D156	I157	E158	G159	W160	R161	W162	M163	L164	G165	L166	A167	V168	V169	P170	S171	V172	I173	L174	L175	V176	G177	I178	Y179	F180	M181	F182	E183	S184	P185	R186	W187	L188	L189	R192	N193	E194	E195	A196	A197	R198	Q199	V200	M201	K202	I203	T204	Y205	D206	D207	S208	E209	I210

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.07Å 118.85Å 160.05Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	19.90 – 3.20 19.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.90-3.20) 98.4 (19.90-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.302 , 0.341 0.296 , 0.338	Depositor DCC
R_{free} test set	1945 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 8.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	16 of 38905 reflections (0.041%)	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.75	1/3258 (0.0%)	0.98	8/4431 (0.2%)
1	B	0.57	0/3258	0.85	4/4431 (0.1%)
All	All	0.67	1/6516 (0.0%)	0.92	12/8862 (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	A	0	2
1	B	0	5
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	TRP	CB-CG	-5.71	1.40	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	GLY	N-CA-C	7.80	132.61	113.10
1	A	39	LEU	CA-CB-CG	6.36	129.92	115.30
1	A	31	LEU	CA-CB-CG	6.32	129.84	115.30
1	A	314	MET	CB-CG-SD	5.95	130.25	112.40
1	B	39	LEU	CA-CB-CG	5.72	128.46	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	PRO	Peptide
1	A	400	THR	Peptide
1	B	206	ASP	Peptide
1	B	233	SER	Peptide
1	B	234	PRO	Peptide

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	3194	0	3399	306	0
1	B	3194	0	3399	262	0
All	All	6388	0	6798	563	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 43.

The worst 5 of 563 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:186:ARG:HG2	1:B:217:MET:HG2	1.32	1.04
1:B:92:SER:HA	1:B:97:LEU:HD11	1.38	1.01
1:A:330:ILE:HA	1:A:333:SER:HB3	1.49	0.94
1:A:324:LEU:HD11	1:A:336:ILE:HB	1.52	0.90
1:A:283:ILE:HD11	1:A:342:SER:HA	1.53	0.89

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	419/446 (94%)	350 (84%)	58 (14%)	11 (3%)	7	40
1	B	419/446 (94%)	355 (85%)	58 (14%)	6 (1%)	14	57
All	All	838/892 (94%)	705 (84%)	116 (14%)	17 (2%)	9	48

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	PRO
1	A	235	TRP
1	B	234	PRO
1	B	328	ILE
1	B	194	GLU

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	341/363 (94%)	256 (75%)	85 (25%)	1	3
1	B	341/363 (94%)	267 (78%)	74 (22%)	1	6
All	All	682/726 (94%)	523 (77%)	159 (23%)	1	4

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	ILE
1	B	37	ILE
1	B	360	LEU
1	A	382	ILE
1	A	405	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	311	ASN

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 [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	421/446 (94%)	1.62	123 (29%) 1 0	10, 149, 347, 447	0
1	B	421/446 (94%)	1.40	104 (24%) 1 1	10, 224, 394, 532	0
All	All	842/892 (94%)	1.51	227 (26%) 1 0	10, 185, 372, 532	0

The worst 5 of 227 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	SER	23.0
1	B	207	ASP	16.3
1	A	427	GLY	15.5
1	B	371	ALA	14.5
1	A	370	GLY	14.4

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 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.