



wwPDB X-ray Structure Validation Summary Report ⓘ

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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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

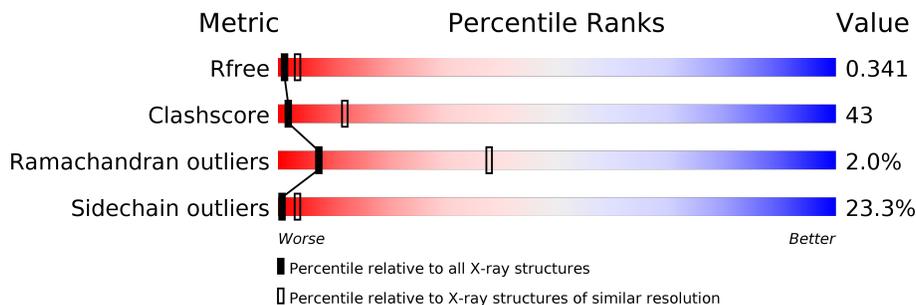
1 Overall quality at a glance

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	446	 30% 49% 14% • 6%
1	B	446	 35% 47% 11% • 6%

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 Glucose transporter GlcP.

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

W235	V298	R367	GLU
L236	D299	L367	LEU
G237	K300	G374	ARG
R238	R303	I375	GLU
I239	K304	S376	ARG
I240	K305	A377	THR
I241	L306	L378	GLY
V242	L307	V379	ALA
G243	V308	N381	ARG
C244	G309	I382	THR
I245	G310	G383	GLU
F246	N311	V387	
A247	I312	S388	
I248	G313	L389	
F249	M314	F390	
Q250	I315	F391	
Q251	F252	P392	
F252	I253	I393	
I253	G254	L317	
G254	I255	L318	
I255	N256	L319	
N256	A257	I320	
A257	V258	M321	
V258	I259	A322	
I259	F260	I323	
F260	Y261	L324	
Y261	S262	I325	
S262	S263	W326	
S263	S264	T327	
S264	I265	I328	
I265	K268	S333	
K268	A269	A334	
A269	G270	W335	
G270	E273	I336	
E273	A274	I337	
A274	A275	I338	
A275	S276	V339	
S276	I277	C340	
I277	L278	L341	
L278	G279	S342	
G279	S280	I345	
S280	V281	V346	
V281	G282	F347	
G282	I283	F348	
I283	G284	G349	
G284	T285	I350	
T285	I286	S351	
I286	M287	W352	
M287	V288	I356	
V288	L289	W357	
L289	V290	V358	
V290	T291	M359	
T291	I292	L360	
I292	V293	P361	
V293	F296	E362	
F296	V297	L363	
V297		TYR	

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)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.302 , 0.341 0.302 , 0.341	Depositor DCC
R_{free} test set	1948 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtrriage
Anisotropy	0.868	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 8.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.11$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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, 0.333 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	0.75	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 [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	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 [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	419/446 (94%)	350 (84%)	58 (14%)	11 (3%)	5	31
1	B	419/446 (94%)	355 (85%)	58 (14%)	6 (1%)	11	46
All	All	838/892 (94%)	705 (84%)	116 (14%)	17 (2%)	7	38

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 [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	341/363 (94%)	256 (75%)	85 (25%)	0	2
1	B	341/363 (94%)	267 (78%)	74 (22%)	1	5
All	All	682/726 (94%)	523 (77%)	159 (23%)	1	3

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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.