Full wwPDB Integrative Structure Validation Report

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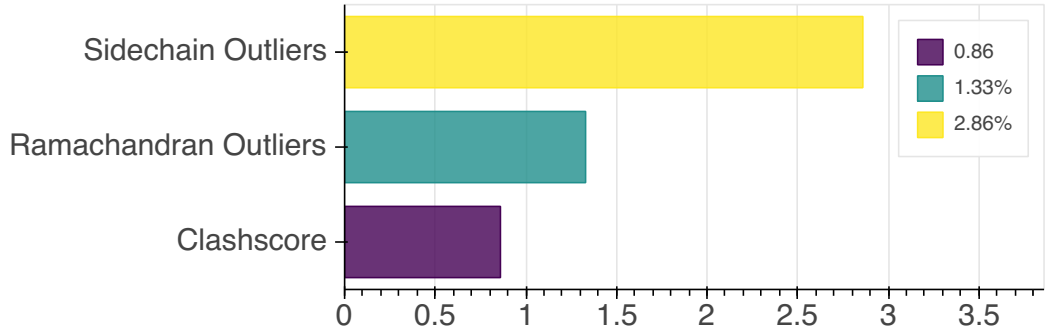
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000031
Molecule Name	Dimer structure of the solute carrier SLC26Dg
Title	Structural basis for functional interactions in dimers of SLC26 transporters
Authors	Chang Y;Jaumann E;Reichel K;Hartmann J;Oliver D;Hummer G;Joseph B;Geertsma E

Overall quality

Model Quality: Molprobity Analysis



Ensemble information

This entry consists of 0 distinct ensemble.

Summary

This entry consists of 1 unique models, with 2 subunits in each model. A total of 2 datasets or restraints was used to build this entry. Each model is represented by 4 rigid bodies and 2 flexible or non-rigid units.

Entry composition

There is 1 unique type of model in this entry.This model is titled Cluster 1/Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	SLC26Dg	A	379
1	2	1	SLC26Dg	B	379

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	?	?	?	False	False

Data quality

Model quality

Standard geometry

There are 5976 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE1--HE1	1.079	0.93	63
CD2--HD2	1.079	0.93	63
NZ--HZ3	1.039	0.89	17
CE2--HE2	1.079	0.93	57
CE3--HE3	1.079	0.93	7
CZ--HZ	1.079	0.93	47
NZ--HZ2	1.039	0.89	17
N--H2	1.041	0.89	1
CD1--HD1	1.079	0.93	65
NZ--HZ1	1.039	0.89	17
CH2--HH2	1.079	0.93	7
N--H3	1.04	0.89	1
CZ2--HZ2	1.08	0.93	7
CZ3--HZ3	1.08	0.93	7
N--H1	1.04	0.89	1
CG2--HG21	1.11	0.97	203
CD1--HD12	1.11	0.97	151
CG2--HG23	1.11	0.97	203
CD2--HD21	1.11	0.97	101
CG--HG3	1.11	0.97	147
CG1--HG12	1.11	0.97	149
CB--HB2	1.11	0.97	487
CB--HB	1.11	0.97	203

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD22	1.11	0.97	101
CG--HG	1.11	0.97	101
CB--HB3	1.11	0.97	481
CG1--HG11	1.11	0.97	99
CD1--HD13	1.11	0.97	151
CD--HD3	1.11	0.97	71
CG1--HG13	1.11	0.97	149
CB--HB1	1.11	0.97	103
CG--HG2	1.11	0.97	147
CG2--HG22	1.11	0.97	203
CD2--HD23	1.11	0.97	101
CD1--HD11	1.11	0.97	151
CE--HE3	1.11	0.97	51
CE--HE1	1.11	0.97	33
CD--HD2	1.11	0.97	71
CE--HE2	1.11	0.97	51
NH2--HH22	0.999	0.86	21
ND2--HD22	0.999	0.86	11
NE--HE	0.999	0.86	21
NH1--HH11	0.999	0.86	21
NH2--HH21	0.999	0.86	21
NE2--HE22	0.999	0.86	27
NE2--HE21	0.999	0.86	27

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--HD21	1.0	0.86	11
NH1--HH12	0.999	0.86	21
ND1--HD1	0.999	0.86	5
N--H	0.996	0.86	717
N--HN	0.996	0.86	5
SG--HG	1.325	1.2	1
OG--HG	0.959	0.84	33
OH--HH	0.959	0.84	9
OG1--HG1	0.959	0.84	53
NE1--HE1	0.976	0.86	7
CA--HA3	1.079	0.97	65
CA--HA	1.079	0.97	691
CA--HA2	1.079	0.97	65

There are 147 angle outliers in this entry.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB3	96.673	109.0	6
CB-CA-HA	96.154	109.0	5
HD21-CD2-HD23	97.398	110.0	2
NE2-CD2-HD2	113.697	126.4	1
CB-CG2-HG23	97.357	110.0	2
HG2-CG-HG3	96.297	110.0	2
CG-CB-HB2	120.468	108.0	3
C-N-H	112.176	124.3	30

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-HA	97.676	110.0	2
HE2-CE-HE3	94.424	110.0	0
HB2-CB-HB3	97.713	110.0	7
HB1-CB-HB3	122.02	110.0	3
HD2-CD-HD3	94.615	110.0	0
CA-N-HN	129.327	114.0	0
HG12-CG1-HG13	97.549	110.0	2
CA-N-H	126.007	114.0	4
HD11-CD1-HD13	97.104	110.0	2
N-CA-HA3	97.28	110.0	1
CB-OG-HG	96.486	110.0	1
HB1-CB-HB2	97.982	110.0	1
N-CA-HA2	97.152	110.0	1
C-CA-HA	96.748	109.0	3
HG21-CG2-HG22	96.639	109.0	1
CD-CG-HG2	120.961	108.0	1
CE-NZ-HZ3	96.018	110.0	0
CB-CG2-HG21	122.855	110.0	1
HD11-CD1-HD12	96.739	110.0	1
HZ1-NZ-HZ2	95.3	109.0	0
CB-CG1-HG11	122.634	109.0	0
CA-CB-HB2	96.806	109.0	2
CB-OG1-HG1	97.762	110.0	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG21-CG2-HG23	97.538	110.0	2
C-CA-HA2	96.238	109.0	1
CD1-CG-HG	121.29	108.0	0
CB-CG1-HG12	95.736	109.0	0
CB-CG1-HG13	122.191	109.0	0
HG22-CG2-HG23	97.663	110.0	1
CB-CG-HG2	122.044	109.0	0
CG-CD2-HD23	121.948	109.0	0
CA-CB-HB	96.108	109.0	0
CG-CD1-HD12	121.846	109.0	0
CG-CD2-HD22	121.624	109.0	1
CB-CG-HG3	96.195	109.0	0
CG-CD2-HD21	121.761	109.0	0
HD21-CD2-HD22	97.293	110.0	0
CZ-NH2-HH21	107.301	120.0	0
HG11-CG1-HG12	97.312	110.0	0
CG-CB-HB3	95.557	108.0	1
CG1-CD1-HD12	121.356	109.0	0
CG1-CB-HB	96.815	109.0	0
SD-CE-HE2	121.147	109.0	0
CD-CG-HG3	120.046	108.0	0
CG-CD2-HD2	138.433	126.4	0
N-CD-HD2	121.015	109.0	0

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
Model 1	0.86	10

All 10 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	754	703	41	10

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:7	ASN
1	A:56	GLY
1	A:132	PRO
1	A:156	PRO
1	A:163	PRO
1	A:190	GLY
1	A:236	ILE
1	B:183	VAL
1	B:236	ILE
1	B:304	GLN

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	594	536	41	17

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:65	THR
1	A:73	THR
1	A:84	LEU
1	A:94	LEU
1	A:111	PRO
1	A:132	PRO
1	A:158	VAL
1	A:193	PRO
1	A:207	THR
1	A:280	THR
1	B:37	PRO
1	B:130	GLN
1	B:138	ASN
1	B:169	ILE
1	B:242	THR
1	B:284	ARG
1	B:347	LEU

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model