

Integrative Structure Validation Report ?

March 27, 2025 - 09:59 AM PDT

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	8ZZV
PDB-Dev ID	PDBDEV_00000031
Structure Title	Dimer structure of the solute carrier SLC26Dg
Structure Authors	Chang Y; Jaumann E; Reichel K; Hartmann J; Oliver D; Hummer G; Joseph B; Geertsma E
Deposited on	2019-03-09

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

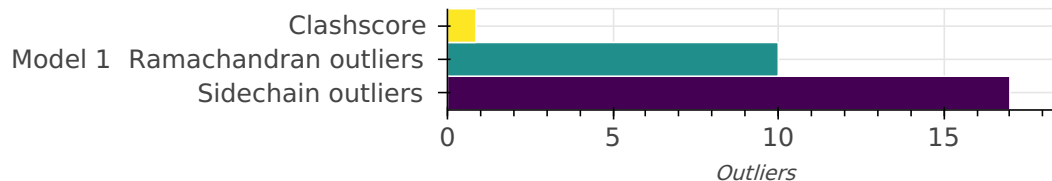
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available [here](#).

Overall quality ?

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 2 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	SLC26Dg	A	379	1-333, 338-379	334-337	100.00 / 98.94	Atomic
				B					

Datasets used for modeling ?

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	5DA0
2	EPR data	Zenodo	10.5281/zenodo.2638061

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	–	–	None	–	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	BioEn	Not available	integrative model building	https://github.com/bio-phys/BioEn

Data quality ?

EPR

Validation for this section is under development.

Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers ?

There are 151 bond length outliers in this entry (2.64% of 5730 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	31	ILE	C-N	8.42	1.45	1.33	1	1
A	198	HIS	ND1-CE1	7.76	1.40	1.32	1	1
B	340	LYS	C-N	7.38	1.43	1.33	1	1
B	367	VAL	C-N	7.09	1.43	1.33	1	1
B	259	VAL	C-N	7.08	1.43	1.33	1	1
A	204	VAL	C-N	7.06	1.23	1.34	1	1
B	222	SER	CA-CB	6.97	1.67	1.53	1	1
A	105	ARG	C-N	6.50	1.42	1.33	1	1
A	165	ALA	C-N	6.32	1.42	1.33	1	1
A	264	GLY	N-CA	6.31	1.55	1.45	1	1
B	284	ARG	CD-NE	6.31	1.55	1.46	1	1
A	251	ARG	CD-NE	6.18	1.54	1.46	1	1
A	75	LEU	C-N	6.11	1.41	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	79	HIS	CB-CG	6.06	1.41	1.50	1	1
B	198	HIS	ND1-CE1	5.94	1.38	1.32	1	1
B	304	GLN	C-N	5.90	1.44	1.34	1	1
A	142	TYR	C-N	5.82	1.41	1.33	1	1
A	321	VAL	C-N	5.79	1.41	1.33	1	1
A	284	ARG	C-N	5.71	1.41	1.33	1	1
B	74	GLY	C-N	5.66	1.41	1.33	1	1
A	164	SER	C-N	5.63	1.41	1.33	1	1
B	198	HIS	CD2-NE2	5.62	1.44	1.37	1	1
B	329	TRP	C-N	5.55	1.41	1.33	1	1
B	248	VAL	C-N	5.55	1.41	1.33	1	1
B	198	HIS	CE1-NE2	5.49	1.27	1.32	1	1
B	372	LEU	C-N	5.48	1.41	1.33	1	1
B	3	GLU	C-N	5.43	1.41	1.33	1	1
A	163	PRO	N-CD	5.41	1.40	1.47	1	1
A	82	GLN	C-N	5.29	1.40	1.33	1	1
B	216	PRO	N-CD	5.29	1.40	1.47	1	1
B	125	LEU	C-N	5.26	1.40	1.33	1	1
B	123	ALA	C-N	5.25	1.40	1.33	1	1
B	254	GLY	CA-C	5.24	1.42	1.52	1	1
A	137	ALA	C-N	5.21	1.40	1.33	1	1
A	255	VAL	C-N	5.18	1.40	1.33	1	1
A	230	LEU	C-N	5.16	1.40	1.33	1	1
A	57	ARG	CD-NE	5.16	1.53	1.46	1	1
B	91	THR	N-CA	5.16	1.56	1.46	1	1
B	101	ALA	C-N	5.13	1.40	1.33	1	1
B	2	ARG	NE-CZ	5.13	1.27	1.33	1	1
A	344	VAL	N-CA	5.11	1.36	1.46	1	1
A	105	ARG	CD-NE	5.06	1.53	1.46	1	1
A	154	LEU	C-N	5.03	1.40	1.33	1	1
A	364	LEU	C-N	5.01	1.40	1.33	1	1
A	15	GLY	C-N	5.01	1.26	1.33	1	1
A	264	GLY	CA-C	5.01	1.43	1.52	1	1
B	210	THR	C-N	5.01	1.40	1.33	1	1
B	36	ASP	CA-C	5.00	1.63	1.52	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	334	THR	C-N	4.99	1.40	1.33	1	1
B	305	PRO	C-N	4.94	1.40	1.33	1	1
B	157	LEU	C-N	4.92	1.40	1.33	1	1
A	299	LEU	C-N	4.91	1.40	1.33	1	1
A	82	GLN	CA-CB	4.90	1.63	1.53	1	1
A	87	ALA	C-N	4.85	1.40	1.33	1	1
A	60	MET	CG-SD	4.85	1.92	1.80	1	1
B	332	LEU	C-N	4.85	1.40	1.33	1	1
B	351	ALA	CA-C	4.83	1.63	1.52	1	1
B	308	VAL	C-N	4.82	1.40	1.33	1	1
A	228	GLU	C-N	4.81	1.40	1.33	1	1
A	130	GLN	C-N	4.81	1.40	1.33	1	1
B	344	VAL	C-N	4.78	1.40	1.33	1	1
B	102	LYS	C-N	4.77	1.40	1.33	1	1
A	202	PRO	N-CD	4.77	1.41	1.47	1	1
B	62	SER	C-N	4.73	1.26	1.33	1	1
A	138	ASN	CA-CB	4.71	1.62	1.53	1	1
A	279	VAL	C-N	4.69	1.39	1.33	1	1
B	279	VAL	C-N	4.69	1.39	1.33	1	1
B	191	THR	CB-OG1	4.69	1.36	1.43	1	1
B	144	MET	CB-CG	4.69	1.66	1.52	1	1
B	139	TRP	C-N	4.67	1.39	1.33	1	1
B	330	GLY	C-N	4.67	1.39	1.33	1	1
B	323	ALA	C-N	4.63	1.39	1.33	1	1
B	290	PHE	C-N	4.61	1.39	1.33	1	1
A	182	ASP	CA-CB	4.59	1.62	1.53	1	1
A	35	VAL	C-N	4.56	1.39	1.33	1	1
B	164	SER	CA-CB	4.56	1.62	1.53	1	1
B	162	MET	CA-CB	4.55	1.62	1.53	1	1
B	172	LEU	C-N	4.54	1.39	1.33	1	1
A	113	SER	CA-CB	4.53	1.62	1.53	1	1
B	124	ILE	C-N	4.53	1.39	1.33	1	1
B	355	PHE	CA-CB	4.53	1.62	1.53	1	1
A	281	SER	C-N	4.52	1.39	1.33	1	1
A	189	MET	CG-SD	4.52	1.92	1.80	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	294	ALA	C-N	4.51	1.39	1.33	1	1
A	169	ILE	CB-CG1	4.50	1.62	1.53	1	1
B	66	GLY	C-N	4.48	1.39	1.33	1	1
A	151	ILE	C-N	4.47	1.39	1.33	1	1
B	251	ARG	CA-CB	4.46	1.62	1.53	1	1
A	122	LEU	C-N	4.46	1.27	1.33	1	1
A	329	TRP	NE1-CE2	4.44	1.42	1.37	1	1
B	51	THR	C-N	4.44	1.39	1.33	1	1
B	5	PHE	C-N	4.43	1.39	1.33	1	1
B	77	LYS	C-N	4.43	1.39	1.33	1	1
A	232	THR	CB-OG1	4.43	1.36	1.43	1	1
B	165	ALA	C-N	4.42	1.39	1.33	1	1
A	127	PHE	CA-CB	4.42	1.62	1.53	1	1
A	185	THR	CA-C	4.41	1.43	1.52	1	1
A	317	ALA	N-CA	4.40	1.54	1.46	1	1
A	57	ARG	CZ-NH1	4.38	1.26	1.32	1	1
B	57	ARG	CD-NE	4.37	1.52	1.46	1	1

Standard geometry: angle outliers ?

There are 350 bond angle outliers in this entry (4.47% of 7822 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	263	PHE	CA-CB-CG	9.33	104.47	113.80	1	1
B	45	PHE	CA-CB-CG	9.22	123.02	113.80	1	1
A	338	PHE	CA-CB-CG	8.92	104.88	113.80	1	1
A	357	HIS	CA-CB-CG	8.68	122.48	113.80	1	1
A	333	ARG	NE-CZ-NH2	8.43	111.61	119.20	1	1
A	23	ILE	CA-C-N	8.35	129.43	116.90	1	1
B	257	ASN	CA-CB-CG	8.35	104.25	112.60	1	1
B	338	PHE	CA-C-N	8.09	129.04	116.90	1	1
A	138	ASN	CA-CB-CG	8.01	120.61	112.60	1	1
B	245	ASP	CA-CB-CG	7.87	120.47	112.60	1	1
A	373	PHE	CA-CB-CG	7.41	121.21	113.80	1	1
B	2	ARG	NE-CZ-NH1	7.24	128.74	121.50	1	1
B	338	PHE	CA-CB-CG	7.22	106.58	113.80	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	138	ASN	CA-CB-CG	7.11	119.71	112.60	1	1
A	373	PHE	N-CA-CB	7.08	98.47	110.50	1	1
A	155	LEU	CA-C-N	7.06	127.48	116.90	1	1
A	131	LEU	CA-C-N	6.89	127.23	116.90	1	1
B	320	MET	CG-SD-CE	6.82	85.90	100.90	1	1
A	204	VAL	CA-C-N	6.81	127.11	116.90	1	1
B	201	PHE	CA-CB-CG	6.78	107.02	113.80	1	1
B	326	THR	OG1-CB-CG2	6.75	95.80	109.30	1	1
A	215	PHE	O-C-N	6.52	112.57	123.00	1	1
B	239	ARG	NE-CZ-NH2	6.52	113.34	119.20	1	1
B	134	PHE	CA-CB-CG	6.51	107.29	113.80	1	1
B	349	THR	CA-CB-OG1	6.33	119.10	109.60	1	1
B	358	ASP	C-CA-CB	6.26	121.99	110.10	1	1
A	112	ARG	NE-CZ-NH1	6.24	115.26	121.50	1	1
A	166	LEU	C-N-CA	6.24	132.92	121.70	1	1
B	92	GLY	C-N-CA	6.23	132.91	121.70	1	1
A	32	ILE	C-N-CA	6.17	132.81	121.70	1	1
A	278	ASN	OD1-CG-ND2	6.17	116.43	122.60	1	1
A	171	VAL	N-CA-CB	6.15	121.96	111.50	1	1
A	201	PHE	CA-C-N	6.12	126.08	116.90	1	1
A	25	GLU	O-C-N	6.07	113.28	123.00	1	1
B	251	ARG	CG-CD-NE	6.04	98.71	112.00	1	1
B	155	LEU	CA-C-N	5.98	125.87	116.90	1	1
A	320	MET	CG-SD-CE	5.97	87.76	100.90	1	1
B	3	GLU	CA-CB-CG	5.96	102.18	114.10	1	1
A	217	VAL	C-N-CA	5.91	132.33	121.70	1	1
A	191	THR	N-CA-CB	5.90	121.53	111.50	1	1
A	42	TYR	CB-CG-CD1	5.90	129.65	120.80	1	1
A	163	PRO	C-N-CA	5.88	132.29	121.70	1	1
B	357	HIS	CD2-NE2-CE1	5.87	103.13	109.00	1	1
B	269	CYS	N-CA-CB	5.85	120.45	110.50	1	1
B	291	VAL	CA-CB-CG1	5.85	120.34	110.40	1	1
B	162	MET	CG-SD-CE	5.80	88.14	100.90	1	1
A	7	ASN	N-CA-CB	5.78	120.32	110.50	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	93	VAL	O-C-N	5.76	113.78	123.00	1	1
A	262	PHE	CA-CB-CG	5.75	108.05	113.80	1	1
A	68	MET	N-CA-CB	5.72	100.77	110.50	1	1
B	212	ALA	C-CA-CB	5.72	119.08	110.50	1	1
A	245	ASP	O-C-N	5.71	113.86	123.00	1	1
A	35	VAL	O-C-N	5.66	113.94	123.00	1	1
B	176	ALA	O-C-N	5.66	113.94	123.00	1	1
A	127	PHE	CA-CB-CG	5.65	119.45	113.80	1	1
B	23	ILE	CA-C-N	5.61	125.32	116.90	1	1
A	198	HIS	CG-CD2-NE2	5.61	112.81	107.20	1	1
B	356	THR	CA-CB-OG1	5.60	118.00	109.60	1	1
B	186	VAL	N-CA-CB	5.59	101.99	111.50	1	1
B	23	ILE	O-C-N	5.59	114.06	123.00	1	1
B	263	PHE	CA-CB-CG	5.58	108.22	113.80	1	1
B	255	VAL	CA-CB-CG2	5.58	100.92	110.40	1	1
B	123	ALA	C-CA-CB	5.57	102.14	110.50	1	1
B	373	PHE	C-CA-CB	5.56	120.67	110.10	1	1
B	255	VAL	CA-CB-CG1	5.53	119.80	110.40	1	1
B	198	HIS	CD2-NE2-CE1	5.52	103.48	109.00	1	1
A	247	ASN	CA-CB-CG	5.51	107.09	112.60	1	1
B	343	THR	OG1-CB-CG2	5.50	98.31	109.30	1	1
B	286	ARG	C-N-CA	5.47	131.55	121.70	1	1
A	342	GLU	N-CA-CB	5.47	119.80	110.50	1	1
B	363	VAL	O-C-N	5.46	114.26	123.00	1	1
B	144	MET	CG-SD-CE	5.45	88.91	100.90	1	1
B	253	GLN	CA-C-O	5.45	130.06	120.80	1	1
B	21	ALA	C-N-CA	5.41	131.44	121.70	1	1
A	377	LYS	N-CA-CB	5.40	119.68	110.50	1	1
A	140	GLN	CB-CG-CD	5.37	103.46	112.60	1	1
B	160	LYS	N-CA-CB	5.37	101.37	110.50	1	1
A	200	GLN	C-N-CA	5.37	131.36	121.70	1	1
A	346	MET	CG-SD-CE	5.36	89.10	100.90	1	1
B	3	GLU	O-C-N	5.36	114.43	123.00	1	1
B	357	HIS	CG-CD2-NE2	5.34	112.54	107.20	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	127	PHE	CA-CB-CG	5.34	119.14	113.80	1	1
B	52	ALA	N-CA-CB	5.34	102.38	110.40	1	1
A	360	SER	CA-CB-OG	5.34	121.78	111.10	1	1
B	349	THR	OG1-CB-CG2	5.34	98.63	109.30	1	1
B	201	PHE	CA-C-N	5.34	124.90	116.90	1	1
B	178	VAL	C-CA-CB	5.32	101.29	111.40	1	1
B	38	GLN	C-N-CA	5.32	131.28	121.70	1	1
A	49	LEU	O-C-N	5.31	114.50	123.00	1	1
A	109	PHE	CA-CB-CG	5.31	108.49	113.80	1	1
A	284	ARG	NE-CZ-NH1	5.29	126.79	121.50	1	1
A	135	VAL	C-N-CA	5.27	131.19	121.70	1	1
B	357	HIS	ND1-CE1-NE2	5.27	113.67	108.40	1	1
B	352	VAL	N-CA-CB	5.27	120.46	111.50	1	1
A	116	VAL	CA-CB-CG2	5.25	101.48	110.40	1	1
B	284	ARG	NE-CZ-NH1	5.25	126.75	121.50	1	1
A	341	GLY	C-N-CA	5.23	131.12	121.70	1	1
B	105	ARG	NE-CZ-NH2	5.23	114.49	119.20	1	1
B	290	PHE	N-CA-CB	5.22	101.62	110.50	1	1
B	338	PHE	O-C-N	5.21	114.66	123.00	1	1

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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	0.86	10

There are 10 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:152:ILE:HG21	A:321:VAL:HG11	0.54	1	1
A:4:TRP:CZ2	A:6:ALA:HB3	0.48	1	1
A:134:PHE:CZ	A:141:MET:HE3	0.47	1	1
B:152:ILE:HD11	B:318:VAL:HG22	0.43	1	1
B:166:LEU:O	B:170:VAL:HG23	0.42	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:276:MET:HB3	B:276:MET:HE3	0.42	1	1
A:83:TYR:CD1	A:204:VAL:HG23	0.42	1	1
A:232:THR:HG21	A:270:ALA:O	0.41	1	1
A:341:GLY:O	A:345:VAL:HG23	0.41	1	1
A:133:GLN:HG3	A:316:VAL:HG21	0.41	1	1

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	Analysed	Favored	Allowed	Outliers
1	754	703	41	10

There are 10 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
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	1

Torsion angles : Protein sidechains ?

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

Model ID	Analysed	Favored	Allowed	Outliers
1	594	536	41	17

There are 17 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	65	THR	1
A	73	THR	1
A	84	LEU	1
A	94	LEU	1

Chain	Res	Type	Models (Total)
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	1

Fit of model to data used for modeling ?

EPR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

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