

Integrative Structure Validation Report

July 22, 2024 - 03:52 PM PDT

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

Python-IHM Version 1.3

MolProbity Version 4.5.2

Integrative Modeling Validation Version 1.2

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

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

We welcome your comments at pdb-dev@mail.wwpdb.org

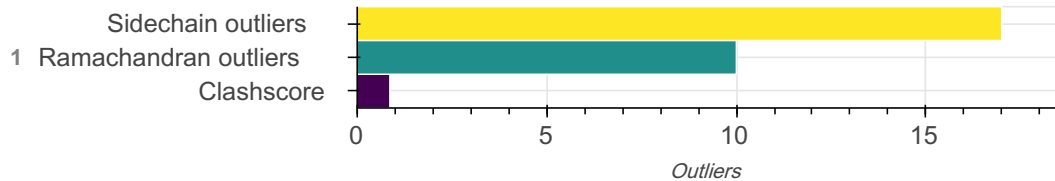
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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 assessment for SAS datasets and fit to model assessments for SAS 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 unique models, with 2 subunits in each model. A total of 2 datasets or restraints were 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 models in this entry. This model is titled Cluster 1/Best scoring model.

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

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	Other	File	10.5281/zenodo.2638061

Representation ?

This entry has only one representation and includes 4 rigid bodies and 2 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-333, 338-3791-333, 338-379	334-337
B	-	334-337

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 ?

Model quality ?

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

Standard geometry: bond outliers ?

There are 5976 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.08	0.97	692
CA--HA2	1.08	0.97	66
CA--HA3	1.08	0.97	66
NE1--HE1	0.98	0.86	8

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OH--HH	0.96	0.84	10
OG1--HG1	0.96	0.84	54
OG--HG	0.96	0.84	34
SG--HG	1.32	1.20	2
N--H	1.00	0.86	718
N--HN	1.00	0.86	6
NE2--HE21	1.00	0.86	28
NH2--HH22	1.00	0.86	22
NH1--HH12	1.00	0.86	22
NE--HE	1.00	0.86	22
ND1--HD1	1.00	0.86	6
ND2--HD22	1.00	0.86	12
NH2--HH21	1.00	0.86	22
NE2--HE22	1.00	0.86	28
NH1--HH11	1.00	0.86	22
ND2--HD21	1.00	0.86	12
CD2--HD21	1.11	0.97	102
CD2--HD22	1.11	0.97	102
CE--HE3	1.11	0.97	52
CG--HG2	1.11	0.97	148
CG--HG3	1.11	0.97	148
CB--HB2	1.11	0.97	488
CB--HB3	1.11	0.97	482

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG2--HG21	1.11	0.97	204
CE--HE2	1.11	0.97	52
CG2--HG22	1.11	0.97	204
CE--HE1	1.11	0.97	34
CD1--HD11	1.11	0.97	152
CB--HB	1.11	0.97	204
CG2--HG23	1.11	0.97	204
CG--HG	1.11	0.97	102
CG1--HG11	1.11	0.97	100
CD1--HD13	1.11	0.97	152
CG1--HG13	1.11	0.97	150
CD1--HD12	1.11	0.97	152
CD2--HD23	1.11	0.97	102
CD--HD2	1.11	0.97	72
CB--HB1	1.11	0.97	104
CG1--HG12	1.11	0.97	150
CD--HD3	1.11	0.97	72
CD2--HD2	1.08	0.93	64
NZ--HZ2	1.04	0.89	18
CE2--HE2	1.08	0.93	58
CZ--HZ	1.08	0.93	48
CE1--HE1	1.08	0.93	58
NZ--HZ1	1.04	0.89	18

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD1	1.08	0.93	66
CH2--HH2	1.08	0.93	8
NZ--HZ3	1.04	0.89	18
CE3--HE3	1.08	0.93	8
CZ2--HZ2	1.08	0.93	8
CZ3--HZ3	1.08	0.93	8
N--H1	1.04	0.89	2
N--H3	1.04	0.89	2
N--H2	1.04	0.89	2
CE1--HE1	1.09	0.93	6

Standard geometry: angle outliers

There are 497 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	104.47	1
CA-CB-CG	113.80	123.02	1
CA-CB-CG	113.80	104.88	1
CA-CB-CG	113.80	122.48	1
NE-CZ-NH2	119.20	111.61	1
CA-C-N	116.90	129.43	1
CA-CB-CG	112.60	104.25	1
CA-C-N	116.90	129.04	1
CA-CB-CG	112.60	120.61	1
CA-CB-CG	112.60	120.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	121.21	1
NE-CZ-NH1	121.50	128.74	1
CA-CB-CG	113.80	106.58	1
CA-CB-CG	112.60	119.71	1
N-CA-CB	110.50	98.47	1
CA-C-N	116.90	127.48	1
CA-C-N	116.90	127.23	1
CG-SD-CE	100.90	85.90	1
CA-C-N	116.90	127.11	1
CA-CB-CG	113.80	107.02	1
OG1-CB-CG2	109.30	95.80	1
O-C-N	123.00	112.57	1
NE-CZ-NH2	119.20	113.34	1
CA-CB-CG	113.80	107.29	1
CA-CB-OG1	109.60	119.10	1
C-CA-CB	110.10	121.99	1
NE-CZ-NH1	121.50	115.26	1
C-N-CA	121.70	132.92	1
C-N-CA	121.70	132.91	1
C-N-CA	121.70	132.81	1
OD1-CG-ND2	122.60	116.43	1
N-CA-CB	111.50	121.96	1
CA-C-N	116.90	126.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	113.28	1
CG-CD-NE	112.00	98.71	1
CA-C-N	116.90	125.87	1
CG-SD-CE	100.90	87.76	1
CA-CB-CG	114.10	102.18	1
C-N-CA	121.70	132.33	1
N-CA-CB	111.50	121.53	1
CB-CG-CD1	120.80	129.65	1
C-N-CA	121.70	132.29	1
CD2-NE2-CE1	109.00	103.13	1
N-CA-CB	110.50	120.45	1
CA-CB-CG1	110.40	120.34	1
CG-SD-CE	100.90	88.14	1
N-CA-CB	110.50	120.32	1
O-C-N	123.00	113.78	1
CA-CB-CG	113.80	108.05	1
N-CA-CB	110.50	100.77	1
C-CA-CB	110.50	119.08	1
O-C-N	123.00	113.86	1
O-C-N	123.00	113.94	2
CA-CB-CG	113.80	119.45	1
CA-C-N	116.90	125.32	1
CG-CD2-NE2	107.20	112.81	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OG1	109.60	118.00	1
N-CA-CB	111.50	101.99	1
O-C-N	123.00	114.06	1
CA-CB-CG	113.80	108.22	1
CA-CB-CG2	110.40	100.92	1
C-CA-CB	110.50	102.14	1
C-CA-CB	110.10	120.67	1
CA-CB-CG1	110.40	119.80	1
CD2-NE2-CE1	109.00	103.48	1
CA-CB-CG	112.60	107.09	1
OG1-CB-CG2	109.30	98.31	1
C-N-CA	121.70	131.55	1
N-CA-CB	110.50	119.80	1
O-C-N	123.00	114.26	1
CG-SD-CE	100.90	88.91	1
CA-C-O	120.80	130.06	1
C-N-CA	121.70	131.44	1
N-CA-CB	110.50	119.68	1
CB-CG-CD	112.60	103.46	1
N-CA-CB	110.50	101.37	1
C-N-CA	121.70	131.36	1
CG-SD-CE	100.90	89.10	1
O-C-N	123.00	114.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD2-NE2	107.20	112.54	1
CA-CB-CG	113.80	119.14	1
N-CA-CB	110.40	102.38	1
CA-CB-OG	111.10	121.78	1
OG1-CB-CG2	109.30	98.63	1
CA-C-N	116.90	124.90	1
C-CA-CB	111.40	101.29	1
C-N-CA	121.70	131.28	1
O-C-N	123.00	114.50	1
CA-CB-CG	113.80	108.49	1
NE-CZ-NH1	121.50	126.79	1
C-N-CA	121.70	131.19	1
ND1-CE1-NE2	108.40	113.67	1
N-CA-CB	111.50	120.46	1
CA-CB-CG2	110.40	101.48	1
NE-CZ-NH1	121.50	126.75	1
C-N-CA	121.70	131.12	1
NE-CZ-NH2	119.20	114.49	1
N-CA-CB	110.50	101.62	1
O-C-N	123.00	114.66	1
C-N-CA	121.70	131.08	1
O-C-N	123.00	114.69	1
CA-CB-CG2	110.50	119.33	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD1	126.90	119.16	1
C-CA-CB	110.10	119.89	1
CA-CB-CG	114.10	124.39	1
CA-CB-OG	111.10	121.38	1
O-C-N	123.00	114.78	1
O-C-N	123.00	114.79	1
O-C-N	123.00	114.80	1
O-C-N	123.00	114.81	1
CA-C-N	116.90	124.52	1
CB-CG-CD	112.60	121.23	1
C-N-CA	121.70	130.83	1
C-CA-CB	110.50	118.11	1
C-N-CA	121.70	130.82	1
O-C-N	123.00	114.97	1
C-CA-CB	110.10	119.63	1
CA-C-N	116.20	126.19	1
CA-CB-CG2	110.50	118.97	1
CA-C-N	116.90	124.35	1
NE-CZ-NH1	121.50	126.47	1
CA-CB-CG1	110.40	118.85	1
CA-CB-CG2	110.40	101.97	1
CD2-NE2-CE1	109.00	104.05	1
O-C-N	123.00	115.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.09	1
O-C-N	123.00	115.11	1
N-CA-CB	110.50	118.86	1
C-CA-CB	110.50	103.14	1
CG-SD-CE	100.90	90.16	1
O-C-N	123.00	115.20	2
C-N-CA	121.70	130.45	1
O-C-N	123.00	115.23	1
C-CA-CB	110.10	119.32	1
CA-C-N	116.20	125.89	1
CB-CG-CD1	126.90	119.64	1
O-C-N	123.00	115.28	1
NH1-CZ-NH2	119.30	113.04	1
O-C-N	123.00	115.29	1
C-CA-CB	110.50	103.28	1
OG1-CB-CG2	109.30	99.69	1
C-CA-CB	110.50	117.71	1
CA-C-N	116.90	124.11	1
C-N-CA	121.70	130.34	1
CG-SD-CE	100.90	90.35	1
N-CA-CB	110.50	118.64	1
C-N-CA	121.70	130.31	1
CG-CD2-NE2	107.20	111.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	119.18	1
CA-CB-OG1	109.60	102.44	1
C-N-CA	121.70	130.29	1
C-N-CA	121.70	130.28	1
CA-CB-CG	114.10	123.63	1
CA-CB-CG	112.60	107.84	1
CA-CB-CG	113.80	109.05	1
N-CA-CB	111.50	119.56	1
C-N-CA	121.70	130.22	1
O-C-N	123.00	115.44	1
CB-CG-CD2	131.20	125.06	1
CA-C-N	116.90	123.96	1
N-CD-CG	103.20	110.26	1
CG-SD-CE	100.90	90.55	1
CD2-CE2-CZ2	122.40	127.10	1
C-N-CA	121.70	130.15	1
OD1-CG-ND2	122.60	117.91	1
CG-CD-NE	112.00	101.71	1
C-N-CA	121.70	130.11	1
O-C-N	123.00	115.53	1
N-CA-C	111.00	124.08	1
C-N-CA	121.70	130.08	1
CA-CB-CG	113.80	109.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CD-CG	103.20	110.18	1
N-CA-CB	111.50	119.40	1
O-C-N	123.00	115.57	1
O-C-N	123.00	115.58	3
C-CA-CB	110.10	118.90	1
C-CA-CB	110.50	117.43	1
CB-CG-CD	112.60	120.44	1
O-C-N	123.00	115.62	1
CB-CG-OD2	118.40	107.83	1
CB-CG-CD	112.60	120.40	1
CA-CB-CG1	110.40	118.19	1
O-C-N	123.00	115.67	1
C-N-CA	121.70	129.95	1
O-C-N	123.00	115.68	1
N-CA-CB	111.50	119.27	1
C-CA-CB	110.10	101.42	1
C-N-CA	121.70	129.91	1
C-CA-CB	110.50	103.68	1
CA-CB-CG	114.10	123.18	1
CA-CB-CG	112.60	108.07	1
OG1-CB-CG2	109.30	100.25	1
CA-CB-CG1	110.40	118.08	1
ND1-CE1-NE2	108.40	112.91	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	102.83	1
CA-C-N	116.90	123.65	1
O-C-N	123.00	115.81	2
CA-CB-CG2	110.40	102.77	1
C-CA-CB	110.10	101.57	1
CB-CG-CD	112.60	104.97	1
N-CA-CB	110.40	103.67	1
CA-CB-OG1	109.60	116.32	1
N-CD-CG	103.20	109.91	1
CB-CG-CD	112.60	105.00	1
CA-C-O	120.80	128.39	1
N-CA-CB	110.40	103.70	1
CA-CB-CG	113.80	109.35	1
C-CA-CB	110.50	103.82	1
OE1-CD-NE2	122.60	118.16	1
CD2-NE2-CE1	109.00	104.56	1
C-N-CA	121.70	129.69	2
CA-CB-CG	112.60	108.17	1
CG1-CB-CG2	110.80	101.05	1
CG-CD-CE	111.30	121.49	1
O-C-N	123.00	115.92	1
CA-CB-CG	112.60	117.01	1
C-CA-CB	110.50	103.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OG1	109.60	116.20	1
CA-CB-CG	114.10	122.87	1
C-N-CA	121.70	129.58	1
CA-CB-CG	113.80	109.42	1
C-N-CA	121.70	129.57	1
CA-C-N	116.90	123.45	1
NE-CZ-NH1	121.50	125.86	1
O-C-N	123.00	129.98	1
O-C-N	123.00	116.02	1
NH1-CZ-NH2	119.30	124.97	1
N-CA-CB	110.50	117.90	1
C-CA-CB	111.60	102.90	1
C-CA-CB	110.10	118.37	1
OE1-CD-NE2	122.60	118.25	1
CB-CG-CD2	120.80	114.28	1
CD-NE-CZ	124.40	130.46	1
C-N-CA	121.70	129.49	1
N-CA-CB	103.00	107.76	1
CA-CB-CG2	110.40	117.75	1
CA-C-O	120.80	128.14	1
CB-CG-CD	112.60	105.26	1
O-C-N	123.00	116.09	1
CA-C-O	120.80	128.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	118.30	1
CA-CB-CG1	110.40	117.73	1
CA-C-N	116.90	123.36	1
NE-CZ-NH1	121.50	125.80	1
CA-CB-CG2	110.40	103.09	1
CG-CD2-CE2	120.70	128.01	1
O-C-N	123.00	116.12	1
C-N-CA	121.70	129.43	1
O-C-N	123.00	116.13	1
CA-CB-CG2	110.40	103.11	1
CA-C-N	116.90	123.32	1
CA-C-N	116.90	123.31	1
O-C-N	123.00	116.16	1
N-CA-CB	111.50	104.23	1
CA-CB-OG1	109.60	116.00	1
C-CA-CB	110.10	118.20	1
CA-C-O	120.80	128.05	1
O-C-N	123.00	116.20	1
C-N-CA	121.70	129.34	1
CA-C-O	120.80	113.58	1
O-C-N	123.00	116.22	1
OE1-CD-NE2	122.60	118.36	1
N-CA-CB	110.50	103.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	116.85	1
CA-CB-CG1	110.40	117.59	1
CA-CB-OG1	109.60	115.94	1
N-CA-C	111.00	122.84	1
CA-CB-CG	113.80	118.03	1
CG1-CB-CG2	110.80	101.50	1
O-C-N	123.00	116.24	1
CA-CB-CG1	110.40	103.22	1
N-CA-CB	110.50	117.68	1
CA-CB-OG1	109.60	115.92	1
NH1-CZ-NH2	119.30	124.77	1
O-C-N	123.00	116.28	2
C-CA-CB	110.10	118.07	1
O-C-N	123.00	129.71	1
O-C-N	123.00	116.29	1
CG-SD-CE	100.90	91.68	1
CA-C-N	116.20	124.57	1
C-CA-CB	111.40	103.45	1
CA-CB-OG1	109.60	115.87	1
O-C-N	123.00	129.68	1
C-N-CA	121.70	129.22	1
C-CA-CB	110.10	118.03	1
C-CA-CB	110.50	104.24	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	117.49	1
CA-CB-CG2	110.40	103.32	1
N-CA-C	112.10	122.50	1
N-CA-CB	103.00	107.57	1
C-N-CA	121.70	129.16	1
O-C-N	123.00	116.37	1
NE-CZ-NH2	119.20	115.48	1
CA-CB-CG1	110.40	117.42	1
C-N-CA	121.70	129.13	1
CD1-CG-CD2	110.80	101.72	1
CA-C-O	120.80	127.81	1
O-C-N	123.00	116.40	1
OG1-CB-CG2	109.30	101.06	1
CG-CD-NE2	116.40	122.57	1
C-CA-CB	110.10	117.92	1
CA-CB-OG1	109.60	115.77	1
O-C-N	123.00	116.43	1
N-CA-CB	111.50	118.47	1
C-N-CA	121.70	129.07	1
CB-CG-CD	112.60	105.64	1
CA-C-O	120.80	113.84	1
CA-C-N	116.20	124.38	1
CB-CG-ND2	116.40	122.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	127.75	1
C-N-CA	121.70	129.06	1
C-N-CA	121.70	129.05	1
CG-CD2-NE2	107.20	111.28	1
CA-C-N	116.20	124.34	1
O-C-N	123.00	116.49	1
N-CA-CB	110.40	116.51	1
NH1-CZ-NH2	119.30	114.01	1
C-CA-CB	110.10	117.80	1
CA-C-N	116.20	124.30	1
C-CA-CB	110.10	117.79	1
CG-CD-NE	112.00	103.09	1
O-C-N	123.00	116.53	1
CA-C-O	120.80	113.93	1
CA-C-O	120.80	127.67	1
CB-CG-CD2	126.80	132.46	1
O-C-N	123.00	116.54	3
C-CA-CB	109.10	117.99	1
C-N-CA	121.70	128.96	1
CA-C-N	116.90	122.95	1
O-C-N	123.00	116.55	1
O-C-N	123.00	116.56	1
C-N-CA	121.70	114.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	116.57	2
N-CA-CB	103.00	107.42	1
CA-CB-CG	113.80	117.81	1
CA-C-N	116.20	124.22	1
CA-CB-CG2	110.40	117.22	1
CA-CB-CG2	110.50	117.31	1
CG-CD2-CE3	133.90	129.89	1
N-CA-CB	103.00	107.41	1
CA-N-H	126.01	114.00	1
N-CD-HD2	121.02	109.00	1
HB1-CB-HB2	97.98	110.00	1
HB1-CB-HB3	122.02	110.00	1
CG-CD2-HD2	138.43	126.40	1
CD-CG-HG3	120.05	108.00	1
C-N-H	112.18	124.30	1
SD-CE-HE2	121.15	109.00	1
C-N-H	112.14	124.30	1
C-N-H	112.12	124.30	1
CG1-CB-HB	96.81	109.00	1
CA-CB-HB2	96.81	109.00	1
CB-OG1-HG1	97.76	110.00	1
C-CA-HA	96.75	109.00	1
HB2-CB-HB3	97.71	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB2-CB-HB3	97.69	110.00	1
N-CA-HA	97.68	110.00	1
CA-CB-HB3	96.67	109.00	1
HG22-CG2-HG23	97.66	110.00	1
CG1-CD1-HD12	121.36	109.00	1
HG21-CG2-HG22	96.64	109.00	1
CA-CB-HB3	96.63	109.00	1
C-N-H	111.91	124.30	1
HB2-CB-HB3	97.56	110.00	1
CG-CB-HB3	95.56	108.00	1
HG12-CG1-HG13	97.55	110.00	1
HG21-CG2-HG23	97.54	110.00	1
CG-CB-HB2	120.47	108.00	1
CA-CB-HB3	121.58	109.00	1
CG-CB-HB2	97.42	110.00	1
CG-CB-HB3	97.42	110.00	1
N-CA-HA	97.40	110.00	1
HB2-CB-HB3	97.40	110.00	1
HD21-CD2-HD23	97.40	110.00	1
C-N-H	111.69	124.30	1
CG-CD2-HD22	121.62	109.00	1
C-N-H	111.66	124.30	1
CB-CG2-HG23	97.36	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB2-CB-HB3	97.33	110.00	1
CA-CB-HB3	121.68	109.00	1
HG11-CG1-HG12	97.31	110.00	1
CZ-NH2-HH21	107.30	120.00	1
NE2-CD2-HD2	113.70	126.40	1
HD21-CD2-HD22	97.29	110.00	1
CB-OG1-HG1	97.29	110.00	1
N-CA-HA3	97.28	110.00	1
HD21-CD2-HD23	97.27	110.00	1
CG-CD2-HD21	121.76	109.00	1
C-CA-HA2	96.24	109.00	1
C-N-H	111.53	124.30	1
C-N-H	111.50	124.30	1
CB-CG-HG3	96.19	109.00	1
C-N-H	111.48	124.30	1
CG-CD2-HD22	121.82	109.00	1
HB1-CB-HB3	97.17	110.00	2
C-N-H	111.47	124.30	1
CG-CD1-HD12	121.85	109.00	1
CB-CA-HA	96.15	109.00	1
N-CA-HA2	97.15	110.00	1
CA-CB-HB2	121.86	109.00	1
CB-CG2-HG21	122.86	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	96.14	109.00	1
CA-CB-HB	96.11	109.00	1
HD11-CD1-HD13	97.10	110.00	1
HD11-CD1-HD13	97.07	110.00	1
CG-CD2-HD23	121.95	109.00	1
C-CA-HA	96.05	109.00	1
CD-CG-HG2	120.96	108.00	1
CA-N-H	126.99	114.00	1
C-N-H	111.27	124.30	1
C-N-H	111.26	124.30	1
CB-CG-HG2	122.04	109.00	1
HG22-CG2-HG23	123.05	110.00	1
C-N-H	111.21	124.30	1
HG12-CG1-HG13	96.91	110.00	1
C-N-H	111.13	124.30	1
CB-CG1-HG13	122.19	109.00	1
C-N-H	111.10	124.30	1
C-N-H	111.07	124.30	1
CB-CA-HA	95.74	109.00	1
HD11-CD1-HD12	96.74	110.00	1
CB-CG1-HG12	95.74	109.00	1
CD1-CG-HG	121.29	108.00	1
HG21-CG2-HG23	96.71	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-OG1-HG1	96.71	110.00	1
C-CA-HA2	95.68	109.00	1
HG21-CG2-HG23	96.58	110.00	1
CB-OG1-HG1	96.51	110.00	1
CA-CB-HB3	95.49	109.00	1
CB-OG-HG	96.49	110.00	1
C-N-H	110.72	124.30	1
CB-CA-HA	95.40	109.00	1
CA-CB-HB2	122.63	109.00	1
CB-CG1-HG11	122.63	109.00	1
CB-CA-HA	95.34	109.00	1
CA-N-H	127.69	114.00	1
HZ1-NZ-HZ2	95.30	109.00	1
HG2-CG-HG3	96.30	110.00	1
HD11-CD1-HD12	96.29	110.00	1
CB-CA-HA	95.28	109.00	1
C-N-H	110.56	124.30	1
CB-CG2-HG21	123.85	110.00	1
C-N-H	110.42	124.30	1
CE-NZ-HZ3	96.02	110.00	1
C-N-H	110.31	124.30	1
CA-CB-HB3	94.99	109.00	1
CD-CG-HG2	124.02	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG2-HG23	123.02	109.00	1
C-N-H	110.21	124.30	1
C-N-H	110.14	124.30	1
HG21-CG2-HG22	124.25	110.00	1
C-N-H	110.03	124.30	1
C-CA-HA	94.69	109.00	1
N-CA-HA2	95.65	110.00	1
HB1-CB-HB2	95.64	110.00	1
C-N-H	109.89	124.30	1
CG-CB-HB2	93.51	108.00	1
HG2-CG-HG3	95.36	110.00	1
HB2-CB-HB3	95.34	110.00	1
CB-OG-HG	95.33	110.00	1
C-N-H	109.63	124.30	1
HB2-CB-HB3	95.27	110.00	1
CA-N-H	128.78	114.00	1
N-CA-HA3	95.20	110.00	1
C-N-H	109.47	124.30	1
C-N-H	109.46	124.30	1
HD11-CD1-HD13	95.11	110.00	1
CA-N-H	128.99	114.00	1
HG12-CG1-HG13	94.97	110.00	1
C-N-H	109.00	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-HN	129.33	114.00	1
HD2-CD-HD3	94.61	110.00	1
HB1-CB-HB3	94.55	110.00	1
HB2-CB-HB3	94.51	110.00	1
HE2-CE-HE3	94.42	110.00	1
C-N-H	108.63	124.30	1
N-CA-HA	94.21	110.00	1
C-N-H	108.45	124.30	1
C-N-H	108.41	124.30	1
CG-CB-HB2	92.05	108.00	1
HG2-CG-HG3	94.02	110.00	1
CB-CG2-HG23	125.04	109.00	1
NE2-CD2-HD2	110.11	126.40	1
HD21-CD2-HD23	93.65	110.00	1
CB-CA-HA	92.53	109.00	1
CA-CB-HB3	91.45	109.00	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 the models in this entry.

Model ID	Clash score	Number of clashes
1	0.86	10

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

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:152:ILE:HG21	A:321:VAL:HG11	0.539

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:4:TRP:CZ2	A:6:ALA:HB3	0.483
1	A:134:PHE:CZ	A:141:MET:HE3	0.471
1	B:152:ILE:HD11	B:318:VAL:HG22	0.426
1	B:166:LEU:O	B:170:VAL:HG23	0.423
1	B:276:MET:HB3	B:276:MET:HE3	0.422
1	A:83:TYR:CD2	A:204:VAL:HG23	0.419
1	A:232:THR:HG21	A:270:ALA:O	0.414
1	A:341:GLY:O	A:345:VAL:HG23	0.413
1	A:133:GLN:HG3	A:316:VAL:HG21	0.407

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

Detailed list of outliers are tabulated below.

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	Analysed	Favored	Allowed	Outliers
1	594	536	41	17

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	65	THR
1	A	73	THR
1	A	84	LEU

Model ID	Chain	Residue ID	Residue type
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 used for validation ?

Validation for this section is under development.

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