

Integrative Structure Validation Report ?

March 27, 2025 - 10:13 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	9A85
PDB-Dev ID	PDBDEV_00000370
Structure Title	Equilibrated 52-mer bacterial gasdermin pore model from Vitiosangium sp.
Structure Authors	Johnson, A.G.; Mayer, M.L.; Schaefer, S.L.; McNamara-Bordewick, N.K.; Hummer, G.; Kranzusch, P.J.
Deposited on	2024-01-25

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

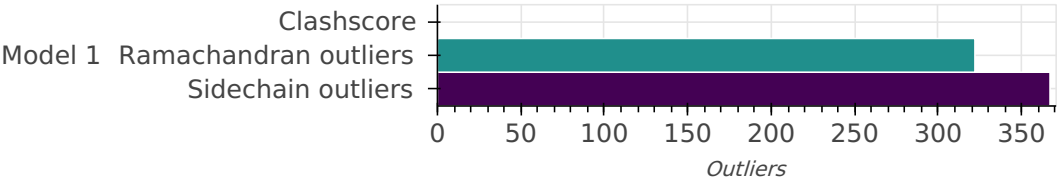
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	Gasdermin bGSDM	A	234	-	1-234	100.00 / 100.00	Atomic
				B					
				C					
				D					
				E					
				F					
				G					
				H					
				I					
				J					
				K					
				L					
				M					
				N					
				O					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				P					
				Q					
				R					
				S					
				T					
				U					
				V					
				W					
				X					
				Y					
				Z					
				AA [a]					
				BA [b]					
				CA [c]					
				DA [d]					
				EA [e]					
				FA [f]					
				GA [g]					
				HA [h]					
				IA [i]					
				JA [j]					
				KA [k]					
				LA [l]					
				MA [m]					
				NA [n]					
				OA [o]					
				PA [p]					
				QA [q]					
				RA [r]					
				SA [s]					
				TA [t]					
				UA [u]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				VA [v]					
				WA [w]					
				XA [x]					
				YA [y]					
				ZA [z]					

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	8sl0
2	Integrative model	PDB	9A84

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	None	This model is derivative of PDB 9A84 and the protocol is therefore highly similar. However, this particular model resulted from allowing the PDB 9A84 model to equilibrate in an MD simulation with backbone positions restrained, but the rest was allowed to move such that key features (i.e., the palmitoyl) entered more natural conformations.	None	False	False

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Python	v3.9.7	model building	https://www.python.org/
2	MDAnalysis	v2.4.2	model building	https://www.mdanalysis.org/
3	Gromacs	v2022.4	MD simulations	https://manual.gromacs.org/2023.4/download.html
4	Charmm	Not available	MD simulations	https://www.charmm.org/

Data quality ?

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 2650 bond length outliers in this entry (2.82% of 93860 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)
JA	4	P1L	SG-C7	365.80	9.05	1.73	1	1
E	4	P1L	SG-C7	363.06	8.99	1.73	1	1
ZA	4	P1L	SG-C7	362.25	8.98	1.73	1	1
G	4	P1L	SG-C7	354.26	8.82	1.73	1	1
L	4	P1L	SG-C7	353.60	8.81	1.73	1	1
F	4	P1L	SG-C7	352.70	8.79	1.73	1	1
P	4	P1L	SG-C7	348.33	8.70	1.73	1	1
TA	4	P1L	SG-C7	345.13	8.64	1.73	1	1
R	4	P1L	SG-C7	342.28	8.58	1.73	1	1
XA	4	P1L	SG-C7	340.79	8.55	1.73	1	1
IA	4	P1L	SG-C7	332.77	8.39	1.73	1	1
Q	4	P1L	SG-C7	332.27	8.38	1.73	1	1
J	4	P1L	SG-C7	332.09	8.37	1.73	1	1
NA	4	P1L	SG-C7	328.80	8.31	1.73	1	1
K	4	P1L	SG-C7	328.06	8.29	1.73	1	1
WA	4	P1L	SG-C7	322.02	8.17	1.73	1	1
N	4	P1L	SG-C7	321.99	8.17	1.73	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
Z	4	P1L	SG-C7	321.63	8.17	1.73	1	1
AA	4	P1L	SG-C7	319.89	8.13	1.73	1	1
W	4	P1L	SG-C7	318.19	8.10	1.73	1	1
O	4	P1L	SG-C7	318.14	8.10	1.73	1	1
D	4	P1L	SG-C7	312.47	7.98	1.73	1	1
OA	4	P1L	SG-C7	311.52	7.96	1.73	1	1
KA	4	P1L	SG-C7	311.28	7.96	1.73	1	1
FA	4	P1L	SG-C7	308.22	7.90	1.73	1	1
YA	4	P1L	SG-C7	302.45	7.78	1.73	1	1
QA	4	P1L	SG-C7	301.34	7.76	1.73	1	1
I	4	P1L	SG-C7	298.57	7.70	1.73	1	1
T	4	P1L	SG-C7	295.96	7.65	1.73	1	1
VA	4	P1L	SG-C7	294.96	7.63	1.73	1	1
SA	4	P1L	SG-C7	292.97	7.59	1.73	1	1
DA	4	P1L	SG-C7	292.56	7.58	1.73	1	1
C	4	P1L	SG-C7	287.70	7.49	1.73	1	1
M	4	P1L	SG-C7	287.20	7.48	1.73	1	1
U	4	P1L	SG-C7	285.06	7.43	1.73	1	1
CA	4	P1L	SG-C7	280.54	7.34	1.73	1	1
UA	4	P1L	SG-C7	276.50	7.26	1.73	1	1
RA	4	P1L	SG-C7	275.65	7.25	1.73	1	1
S	4	P1L	SG-C7	270.94	7.15	1.73	1	1
MA	4	P1L	SG-C7	270.21	7.14	1.73	1	1
V	4	P1L	SG-C7	266.93	7.07	1.73	1	1
PA	4	P1L	SG-C7	264.99	7.03	1.73	1	1
EA	4	P1L	SG-C7	263.18	7.00	1.73	1	1
HA	4	P1L	SG-C7	261.96	6.97	1.73	1	1
B	4	P1L	SG-C7	252.43	6.78	1.73	1	1
GA	4	P1L	SG-C7	228.58	6.30	1.73	1	1
H	4	P1L	SG-C7	220.92	6.15	1.73	1	1
X	4	P1L	SG-C7	216.13	6.06	1.73	1	1
Y	4	P1L	SG-C7	199.69	5.73	1.73	1	1
LA	4	P1L	SG-C7	177.10	5.27	1.73	1	1
A	4	P1L	SG-C7	158.22	4.90	1.73	1	1
BA	4	P1L	SG-C7	120.07	4.13	1.73	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
H	207	GLY	C-N	10.77	1.48	1.33	1	1
ZA	37	ARG	C-N	9.13	1.46	1.33	1	1
B	31	HIS	ND1-CE1	9.13	1.41	1.32	1	1
Q	31	HIS	CB-CG	8.50	1.62	1.50	1	1
I	151	ARG	CD-NE	8.43	1.58	1.46	1	1
A	8	ALA	C-N	8.37	1.45	1.33	1	1
I	125	ALA	C-N	8.25	1.44	1.33	1	1
X	55	SER	C-N	8.13	1.44	1.33	1	1
Y	233	GLN	C-N	8.07	1.44	1.33	1	1
Q	148	GLY	C-N	8.02	1.44	1.33	1	1
T	137	ALA	C-N	8.00	1.44	1.33	1	1
V	37	ARG	CD-NE	7.97	1.57	1.46	1	1
GA	31	HIS	CB-CG	7.91	1.61	1.50	1	1
XA	149	ASN	CA-CB	7.86	1.69	1.53	1	1
XA	223	LYS	C-N	7.85	1.44	1.33	1	1
CA	9	ILE	C-N	7.64	1.44	1.33	1	1
OA	148	GLY	C-N	7.64	1.44	1.33	1	1
X	175	SER	C-N	7.60	1.44	1.33	1	1
J	65	ALA	C-N	7.59	1.44	1.33	1	1
SA	14	ARG	CD-NE	7.54	1.56	1.46	1	1
O	198	SER	C-N	7.49	1.43	1.33	1	1
J	55	SER	C-N	7.48	1.43	1.33	1	1
TA	89	VAL	C-N	7.48	1.43	1.33	1	1
EA	183	ILE	C-N	7.45	1.43	1.33	1	1
CA	213	PHE	C-N	7.44	1.43	1.33	1	1
H	229	LEU	C-N	7.44	1.43	1.33	1	1
K	230	PHE	CA-CB	7.43	1.68	1.53	1	1
RA	37	ARG	C-N	7.43	1.43	1.33	1	1
RA	24	ARG	CD-NE	7.42	1.56	1.46	1	1
L	226	GLU	C-N	7.38	1.43	1.33	1	1
CA	140	PRO	C-N	7.36	1.43	1.33	1	1
HA	130	LEU	C-N	7.35	1.43	1.33	1	1
ZA	48	LYS	C-N	7.32	1.43	1.33	1	1
PA	128	GLN	CA-CB	7.28	1.68	1.53	1	1
P	4	P1L	CB-SG	7.27	1.92	1.77	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
Z	184	GLN	C-N	7.24	1.43	1.33	1	1
WA	62	ARG	CD-NE	7.18	1.56	1.46	1	1
P	29	PRO	N-CD	7.15	1.37	1.47	1	1
LA	31	HIS	ND1-CE1	7.14	1.39	1.32	1	1
WA	100	GLU	C-N	7.13	1.43	1.33	1	1
SA	61	THR	C-N	7.12	1.43	1.33	1	1
FA	14	ARG	CD-NE	7.10	1.56	1.46	1	1
XA	96	GLY	N-CA	7.09	1.56	1.45	1	1
TA	58	PRO	C-N	7.08	1.43	1.33	1	1
OA	52	GLN	C-N	7.07	1.23	1.34	1	1
XA	213	PHE	C-N	7.05	1.43	1.33	1	1
RA	3	LEU	CA-CB	7.05	1.67	1.53	1	1
DA	60	ILE	C-N	7.05	1.43	1.33	1	1

Standard geometry: angle outliers ?

There are 5540 bond angle outliers in this entry (4.37% of 126672 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)
C	4	P1L	SG-C7-C8	23.09	178.50	109.23	1	1
HA	4	P1L	CB-SG-C7	22.08	172.35	106.10	1	1
Y	4	P1L	SG-C7-C8	22.02	175.29	109.23	1	1
OA	4	P1L	CB-SG-C7	21.96	171.98	106.10	1	1
UA	4	P1L	SG-C7-C8	20.77	171.55	109.23	1	1
QA	4	P1L	CB-SG-C7	19.83	165.58	106.10	1	1
DA	4	P1L	CB-SG-C7	19.78	165.43	106.10	1	1
Z	4	P1L	CB-SG-C7	19.38	164.23	106.10	1	1
D	4	P1L	CB-SG-C7	18.56	161.77	106.10	1	1
OA	4	P1L	SG-C7-C8	18.38	164.37	109.23	1	1
SA	4	P1L	SG-C7-C8	18.34	164.26	109.23	1	1
O	4	P1L	CB-SG-C7	17.69	159.16	106.10	1	1
IA	4	P1L	SG-C7-C8	17.14	160.65	109.23	1	1
EA	4	P1L	CB-SG-C7	16.72	156.25	106.10	1	1
C	4	P1L	CB-SG-C7	16.44	155.42	106.10	1	1
D	4	P1L	SG-C7-C8	15.83	156.73	109.23	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
Z	4	P1L	SG-C7-C8	15.78	156.58	109.23	1	1
QA	4	P1L	SG-C7-C8	15.43	155.53	109.23	1	1
KA	4	P1L	CB-SG-C7	15.27	151.91	106.10	1	1
YA	104	ASN	CA-CB-CG	14.66	127.26	112.60	1	1
NA	4	P1L	CB-SG-C7	14.61	149.92	106.10	1	1
O	4	P1L	SG-C7-C8	14.28	152.07	109.23	1	1
HA	4	P1L	SG-C7-C8	14.27	152.04	109.23	1	1
M	4	P1L	CB-SG-C7	13.99	148.08	106.10	1	1
FA	4	P1L	CB-SG-C7	13.71	147.22	106.10	1	1
Q	4	P1L	CB-SG-C7	13.44	146.41	106.10	1	1
KA	21	ARG	NE-CZ-NH2	12.58	107.88	119.20	1	1
S	4	P1L	SG-C7-C8	12.56	71.55	109.23	1	1
X	218	PHE	CA-CB-CG	12.18	101.62	113.80	1	1
F	4	P1L	CB-SG-C7	11.88	141.73	106.10	1	1
L	4	P1L	SG-C7-C8	11.77	144.55	109.23	1	1
V	4	P1L	SG-C7-C8	11.67	144.24	109.23	1	1
PA	4	P1L	SG-C7-C8	11.50	143.74	109.23	1	1
F	53	PRO	CA-C-N	11.35	133.92	116.90	1	1
U	4	P1L	SG-C7-C8	11.30	143.13	109.23	1	1
UA	92	GLN	OE1-CD-NE2	11.26	111.34	122.60	1	1
NA	218	PHE	CA-CB-CG	11.12	102.68	113.80	1	1
FA	4	P1L	SG-C7-C8	11.07	76.01	109.23	1	1
H	4	P1L	SG-C7-C8	11.06	76.05	109.23	1	1
AA	4	P1L	CB-SG-C7	11.02	139.16	106.10	1	1
J	14	ARG	NE-CZ-NH1	11.01	132.51	121.50	1	1
K	24	ARG	NE-CZ-NH1	10.82	132.32	121.50	1	1
W	4	P1L	SG-C7-C8	10.78	76.88	109.23	1	1
K	4	P1L	SG-C7-C8	10.62	141.10	109.23	1	1
M	14	ARG	NE-CZ-NH2	10.59	109.67	119.20	1	1
D	93	PHE	CA-CB-CG	10.53	124.33	113.80	1	1
I	4	P1L	CB-SG-C7	10.44	137.43	106.10	1	1
RA	115	ASN	CA-CB-CG	10.28	122.88	112.60	1	1
CA	76	ASN	CA-CB-CG	10.18	122.78	112.60	1	1
JA	115	ASN	CA-CB-CG	9.94	122.54	112.60	1	1
GA	110	ARG	NE-CZ-NH1	9.94	131.44	121.50	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
FA	14	ARG	NE-CZ-NH1	9.92	131.42	121.50	1	1
EA	37	ARG	NE-CZ-NH1	9.83	131.33	121.50	1	1
Y	53	PRO	CA-C-N	9.82	131.64	116.90	1	1
MA	151	ARG	NE-CZ-NH1	9.75	131.25	121.50	1	1
CA	119	ASP	CA-CB-CG	9.75	102.85	112.60	1	1
Y	62	ARG	NE-CZ-NH1	9.73	131.23	121.50	1	1
Z	113	PHE	CA-CB-CG	9.67	104.13	113.80	1	1
UA	53	PRO	CA-C-N	9.63	131.34	116.90	1	1
HA	21	ARG	NE-CZ-NH1	9.62	131.12	121.50	1	1
MA	128	GLN	OE1-CD-NE2	9.60	113.00	122.60	1	1
Q	62	ARG	NE-CZ-NH2	9.58	110.57	119.20	1	1
YA	179	ASP	CA-CB-CG	9.51	122.11	112.60	1	1
E	113	PHE	CA-CB-CG	9.41	104.39	113.80	1	1
UA	37	ARG	NE-CZ-NH2	9.39	110.75	119.20	1	1
P	6	ASP	CA-CB-CG	9.38	121.98	112.60	1	1
WA	104	ASN	CA-CB-CG	9.38	103.22	112.60	1	1
X	11	TYR	N-CA-CB	9.37	126.43	110.50	1	1
CA	6	ASP	CA-CB-CG	9.36	121.96	112.60	1	1
J	179	ASP	CA-CB-CG	9.33	121.93	112.60	1	1
IA	24	ARG	NE-CZ-NH2	9.32	110.81	119.20	1	1
XA	104	ASN	OD1-CG-ND2	9.32	113.28	122.60	1	1
L	4	P1L	CB-SG-C7	9.24	133.81	106.10	1	1
Q	37	ARG	NE-CZ-NH1	9.21	130.71	121.50	1	1
SA	72	GLN	OE1-CD-NE2	9.15	113.45	122.60	1	1
J	4	P1L	CB-SG-C7	9.13	133.50	106.10	1	1
K	184	GLN	OE1-CD-NE2	9.13	113.47	122.60	1	1
JA	4	P1L	SG-C7-C8	9.08	136.46	109.23	1	1
AA	115	ASN	CA-CB-CG	9.05	121.65	112.60	1	1
V	6	ASP	CA-CB-CG	9.02	121.62	112.60	1	1
ZA	104	ASN	OD1-CG-ND2	8.97	113.63	122.60	1	1
N	128	GLN	OE1-CD-NE2	8.91	113.69	122.60	1	1
DA	213	PHE	CA-CB-CG	8.90	122.70	113.80	1	1
S	105	GLN	OE1-CD-NE2	8.87	113.73	122.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
I	70	ASN	CA-CB-CG	8.83	121.43	112.60	1	1
X	119	ASP	CA-CB-CG	8.82	121.42	112.60	1	1
WA	6	ASP	CA-C-N	8.79	130.09	116.90	1	1
DA	70	ASN	CA-CB-CG	8.74	121.34	112.60	1	1
Y	185	LYS	C-N-CA	8.73	137.42	121.70	1	1
VA	84	ASN	CA-CB-CG	8.70	103.90	112.60	1	1
LA	6	ASP	CA-C-N	8.70	129.95	116.90	1	1
CA	4	P1L	SG-C7-C8	8.69	135.31	109.23	1	1
Q	157	GLN	OE1-CD-NE2	8.67	113.93	122.60	1	1
KA	57	PRO	CA-C-N	8.66	129.89	116.90	1	1
B	107	ARG	NE-CZ-NH1	8.61	130.11	121.50	1	1
M	110	ARG	NE-CZ-NH1	8.61	130.11	121.50	1	1
M	84	ASN	CA-CB-CG	8.61	121.21	112.60	1	1
N	4	P1L	SG-C7-C8	8.61	83.40	109.23	1	1
V	62	ARG	NE-CZ-NH2	8.59	111.46	119.20	1	1
SA	218	PHE	CA-CB-CG	8.58	105.22	113.80	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	0.95	175

There are 175 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
I:28:GLN:HE21	I:31:HIS:CE1	0.66	1	1
BA:28:GLN:H	BA:31:HIS:CE1	0.66	1	1
KA:17:TYR:CE1	LA:22:LEU:HD23	0.62	1	1
ZA:183:ILE:HB	ZA:187:VAL:HG22	0.62	1	1
B:28:GLN:H	B:31:HIS:CE1	0.61	1	1
D:183:ILE:HG22	D:185:LYS:H	0.58	1	1
L:183:ILE:HG22	L:185:LYS:H	0.58	1	1
V:111:PHE:HB3	V:166:VAL:HG23	0.57	1	1
QA:65:ALA:HB2	RA:209:LYS:HE3	0.57	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
SA:24:ARG:O	SA:212:VAL:HG22	0.57	1	1
D:62:ARG:HE	D:119:ASP:CG	0.56	1	1
F:205:TYR:CE2	F:211:LEU:HD13	0.56	1	1
J:75:GLU:HG2	K:197:VAL:HG23	0.56	1	1
NA:67:ALA:H	OA:211:LEU:CD2	0.55	1	1
IA:62:ARG:HE	IA:119:ASP:CG	0.55	1	1
OA:28:GLN:H	OA:31:HIS:CE1	0.54	1	1
K:222:VAL:HG12	K:227:ILE:CD	0.54	1	1
AA:17:TYR:CD2	AA:216:LYS:HG3	0.54	1	1
FA:62:ARG:HE	FA:119:ASP:CG	0.54	1	1
SA:183:ILE:HG22	SA:185:LYS:H	0.54	1	1
C:62:ARG:HE	C:119:ASP:CG	0.53	1	1
UA:124:LEU:HD11	VA:32:LEU:HD23	0.53	1	1
JA:229:LEU:HD12	KA:140:PRO:HG2	0.53	1	1
NA:60:ILE:HG22	NA:62:ARG:HD2	0.52	1	1
L:87:LYS:HG3	M:186:VAL:HG21	0.51	1	1
F:67:ALA:H	G:211:LEU:HD21	0.51	1	1
KA:67:ALA:H	LA:211:LEU:HD21	0.51	1	1
V:50:ILE:HG23	V:133:ALA:HB1	0.51	1	1
M:119:ASP:CG	M:160:LYS:HZ3	0.50	1	1
GA:118:ALA:HB2	GA:159:ILE:HG22	0.50	1	1
M:231:ALA:HB3	N:36:GLN:HG3	0.50	1	1
KA:62:ARG:HE	KA:119:ASP:CG	0.50	1	1
SA:100:GLU:HB2	SA:177:GLN:HE21	0.50	1	1
K:113:PHE:CE1	K:213:PHE:CD2	0.50	1	1
M:7:PRO:HB3	M:73:LYS:HD3	0.50	1	1
KA:87:LYS:HG3	LA:186:VAL:HG21	0.49	1	1
OA:67:ALA:HA	PA:205:TYR:HB2	0.49	1	1
G:210:GLN:C	G:211:LEU:HD12	0.49	1	1
SA:27:ILE:HA	SA:31:HIS:CE1	0.49	1	1
GA:79:PHE:CZ	GA:103:TYR:HB3	0.48	1	1
IA:18:ASN:O	IA:214:GLY:HA2	0.48	1	1
GA:27:ILE:HB	GA:212:VAL:HG21	0.48	1	1
FA:66:ALA:HB3	FA:116:VAL:HG12	0.48	1	1
GA:124:LEU:HD11	HA:32:LEU:HD23	0.48	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
YA:62:ARG:HE	YA:119:ASP:CG	0.48	1	1
HA:124:LEU:HD11	IA:32:LEU:HD23	0.48	1	1
XA:157:GLN:HB3	XA:216:LYS:HB2	0.48	1	1
K:157:GLN:HE22	L:24:ARG:CZ	0.47	1	1
G:35:GLN:HA	G:39:THR:O	0.47	1	1
K:27:ILE:HB	K:212:VAL:HG21	0.47	1	1
DA:68:GLY:HA2	DA:116:VAL:HG21	0.47	1	1
AA:113:PHE:CE2	AA:213:PHE:CD1	0.47	1	1
MA:46:LEU:HD21	MA:126:VAL:HG13	0.47	1	1
WA:43:LEU:HD22	WA:141:VAL:HG11	0.47	1	1
GA:220:ILE:HA	GA:229:LEU:HD23	0.47	1	1
VA:118:ALA:HB2	VA:159:ILE:HG22	0.47	1	1
K:3:LEU:N	K:3:LEU:HD23	0.47	1	1
X:67:ALA:H	Y:211:LEU:HD21	0.47	1	1
U:6:ASP:CG	U:170:LYS:HZ1	0.46	1	1
JA:28:GLN:H	JA:31:HIS:CD2	0.46	1	1
F:184:GLN:CD	F:184:GLN:H	0.46	1	1
N:78:SER:HA	N:104:ASN:HA	0.46	1	1
S:24:ARG:HA	S:211:LEU:HD23	0.46	1	1
GA:205:TYR:CZ	GA:207:GLY:HA3	0.46	1	1
J:24:ARG:O	J:212:VAL:HG22	0.46	1	1
VA:71:GLY:HA2	WA:200:GLN:HE22	0.46	1	1
EA:184:GLN:CD	EA:184:GLN:H	0.46	1	1
J:205:TYR:CE2	J:211:LEU:HD13	0.46	1	1
BA:81:ILE:HA	CA:191:LEU:HB3	0.46	1	1
PA:33:LEU:HD12	PA:40:VAL:HG12	0.46	1	1
VA:18:ASN:HB2	VA:215:PHE:CE1	0.46	1	1
Y:23:PRO:HD2	Y:203:VAL:HG11	0.46	1	1
HA:124:LEU:HD13	IA:48:LYS:HB2	0.46	1	1
IA:109:VAL:HG23	IA:168:ALA:HB2	0.46	1	1
J:123:PRO:HG3	J:156:THR:HG21	0.45	1	1
B:29:PRO:HA	B:155:ILE:HG22	0.45	1	1
D:72:GLN:HB3	D:110:ARG:HA	0.45	1	1
X:67:ALA:H	Y:211:LEU:CD2	0.45	1	1
K:67:ALA:HA	L:205:TYR:CD1	0.45	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
UA:132:MET:HA	UA:132:MET:HE2	0.45	1	1
PA:113:PHE:CD2	PA:164:PHE:HB3	0.45	1	1
A:111:PHE:HB3	A:166:VAL:HG23	0.45	1	1
OA:35:GLN:HB2	OA:40:VAL:HG22	0.45	1	1
L:28:GLN:HB2	L:31:HIS:CE1	0.44	1	1
Z:66:ALA:HB3	Z:116:VAL:HG12	0.44	1	1
CA:160:LYS:HB3	CA:212:VAL:HG12	0.44	1	1
NA:72:GLN:HB2	NA:109:VAL:O	0.44	1	1
TA:231:ALA:HB1	UA:41:GLU:HG3	0.44	1	1
T:124:LEU:HD21	U:142:LEU:HD21	0.44	1	1
VA:17:TYR:CD2	VA:216:LYS:HG3	0.44	1	1
MA:151:ARG:HH21	MA:219:GLU:CD	0.44	1	1
M:231:ALA:HB3	N:36:GLN:CG	0.44	1	1
HA:28:GLN:H	HA:31:HIS:CE1	0.44	1	1
VA:65:ALA:HB2	WA:209:LYS:HD3	0.44	1	1
JA:160:LYS:HA	JA:212:VAL:HA	0.44	1	1
LA:72:GLN:O	MA:199:SER:HB2	0.44	1	1
NA:27:ILE:HB	NA:212:VAL:HG21	0.44	1	1
NA:123:PRO:HG3	NA:156:THR:HG21	0.44	1	1
I:67:ALA:HA	J:205:TYR:CD1	0.43	1	1
K:28:GLN:HB2	K:31:HIS:CE1	0.43	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	11856	10576	958	322

There are 322 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	89	VAL	1
A	92	GLN	1
A	182	GLU	1
A	183	ILE	1
A	186	VAL	1

Chain	Res	Type	Models (Total)
AA	29	PRO	1
AA	67	ALA	1
AA	89	VAL	1
AA	130	LEU	1
AA	183	ILE	1
AA	186	VAL	1
B	22	LEU	1
B	57	PRO	1
B	58	PRO	1
B	67	ALA	1
B	89	VAL	1
B	96	GLY	1
B	131	LYS	1
B	183	ILE	1
B	185	LYS	1
B	186	VAL	1
BA	22	LEU	1
BA	67	ALA	1
BA	92	GLN	1
BA	96	GLY	1
BA	131	LYS	1
BA	183	ILE	1
C	2	GLY	1
C	23	PRO	1
C	55	SER	1
C	57	PRO	1
C	89	VAL	1
C	96	GLY	1
C	182	GLU	1
C	183	ILE	1
C	186	VAL	1
CA	23	PRO	1
CA	58	PRO	1
CA	89	VAL	1
CA	92	GLN	1

Chain	Res	Type	Models (Total)
CA	115	ASN	1
CA	131	LYS	1
CA	183	ILE	1
CA	186	VAL	1
D	55	SER	1
D	89	VAL	1
D	130	LEU	1
D	182	GLU	1
D	183	ILE	1
D	186	VAL	1
DA	22	LEU	1
DA	89	VAL	1
DA	95	ALA	1
DA	132	MET	1
DA	183	ILE	1
E	30	LEU	1
E	89	VAL	1
E	183	ILE	1
E	223	LYS	1
EA	23	PRO	1
EA	59	ALA	1
EA	90	LEU	1
EA	92	GLN	1
EA	96	GLY	1
EA	131	LYS	1
EA	183	ILE	1
F	55	SER	1
F	89	VAL	1
F	131	LYS	1
F	183	ILE	1
F	223	LYS	1
FA	22	LEU	1
FA	89	VAL	1
FA	92	GLN	1
FA	181	PRO	1

Chain	Res	Type	Models (Total)
FA	183	ILE	1
G	22	LEU	1
G	131	LYS	1
G	183	ILE	1
G	186	VAL	1
G	206	LYS	1
G	223	LYS	1
GA	22	LEU	1
GA	45	SER	1
GA	89	VAL	1
GA	96	GLY	1
GA	182	GLU	1
GA	183	ILE	1
GA	206	LYS	1
H	29	PRO	1
H	57	PRO	1
H	92	GLN	1
H	131	LYS	1
H	183	ILE	1
HA	22	LEU	1
HA	30	LEU	1
HA	89	VAL	1
HA	92	GLN	1
HA	131	LYS	1
HA	183	ILE	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	9100	7911	822	367

There are 367 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	7	PRO	1

Chain	Res	Type	Models (Total)
A	19	VAL	1
A	57	PRO	1
A	104	ASN	1
A	165	THR	1
A	184	GLN	1
A	197	VAL	1
A	203	VAL	1
A	212	VAL	1
AA	30	LEU	1
AA	58	PRO	1
AA	76	ASN	1
AA	88	SER	1
AA	115	ASN	1
AA	228	THR	1
B	3	LEU	1
B	23	PRO	1
B	30	LEU	1
B	39	THR	1
B	54	PRO	1
B	135	VAL	1
B	186	VAL	1
B	230	PHE	1
BA	23	PRO	1
BA	35	GLN	1
BA	184	GLN	1
BA	191	LEU	1
BA	197	VAL	1
BA	228	THR	1
BA	230	PHE	1
C	28	GLN	1
C	35	GLN	1
C	47	GLU	1
C	158	VAL	1
C	186	VAL	1
CA	156	THR	1

Chain	Res	Type	Models (Total)
CA	166	VAL	1
CA	181	PRO	1
CA	184	GLN	1
CA	212	VAL	1
D	76	ASN	1
D	90	LEU	1
D	108	LYS	1
D	109	VAL	1
D	154	VAL	1
D	158	VAL	1
D	203	VAL	1
D	212	VAL	1
DA	186	VAL	1
DA	191	LEU	1
DA	212	VAL	1
DA	222	VAL	1
E	23	PRO	1
E	88	SER	1
E	104	ASN	1
E	166	VAL	1
E	177	GLN	1
E	204	THR	1
E	212	VAL	1
EA	47	GLU	1
EA	58	PRO	1
EA	166	VAL	1
EA	191	LEU	1
EA	204	THR	1
EA	208	GLU	1
EA	218	PHE	1
F	3	LEU	1
F	30	LEU	1
F	53	PRO	1
F	58	PRO	1
F	104	ASN	1

Chain	Res	Type	Models (Total)
F	191	LEU	1
F	197	VAL	1
F	204	THR	1
F	218	PHE	1
FA	102	GLN	1
FA	184	GLN	1
FA	186	VAL	1
FA	200	GLN	1
FA	218	PHE	1
G	47	GLU	1
G	70	ASN	1
G	154	VAL	1
G	200	GLN	1
GA	19	VAL	1
GA	23	PRO	1
GA	30	LEU	1
GA	58	PRO	1
GA	76	ASN	1
GA	104	ASN	1
GA	200	GLN	1
GA	203	VAL	1
GA	222	VAL	1
H	61	THR	1
H	158	VAL	1
H	179	ASP	1
H	218	PHE	1
HA	3	LEU	1
HA	7	PRO	1
HA	39	THR	1

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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