

# Integrative Structure Validation Report

July 22, 2024 - 04:12 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	9A00
PDB-Dev ID	PDBDEV_00000060
Structure Title	Integrative structure of Pg-GAFab complex
Structure Authors	Gupta R; Liu Y; Wang H; Nordyke CT; Puterbaugh RZ; Cui W; Varga K; Chu F; Ke H; Vashisth H; Cote RH

*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](mailto:pdb-dev@mail.wwpdb.org)*

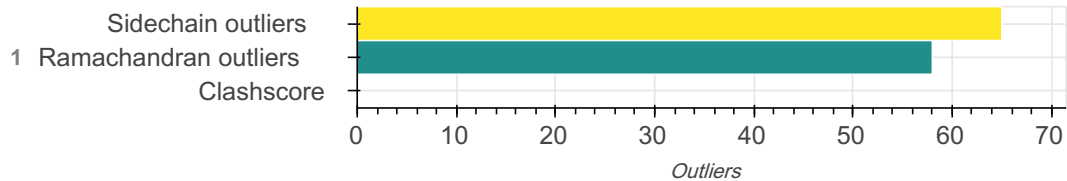
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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 4 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 4 flexible or non-rigid units.

## Entry composition ?

There is 1 unique type of models in this entry. This model is titled None/Best scoring model.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	PDE GAFab	A	A	399
1	2	1	PDE GAFab	B	B	399
1	3	2	PDE gamma subunit	C	C	51
1	4	2	PDE gamma subunit	D	D	51

## Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD020817
2	Experimental model	PDB	6X88

ID	Dataset type	Database name	Data access code
3	Integrative model	PDB-Dev	PDBDEV_00000059

## Representation ?

*This entry has only one representation and includes 0 rigid bodies and 4 flexible units*

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-399
B	-	1-399
C	-	1-51
D	-	1-51

## 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	None	None	False	False

*There are 2 software packages reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="https://integrativemodeling.org">Integrative Modeling Platform (IMP)</a>	Not available	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
2	<a href="https://salilab.org/modeller/">Modeller</a>	Not available	model building	<a href="https://salilab.org/modeller/">https://salilab.org/modeller/</a>

## Data quality ?

[Crosslinking-MS](#)

Validation for this section is under development.

### Model quality ?

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

#### Standard geometry: bond outliers ?

*Bond length outliers can not be evaluated for this model*

#### Standard geometry: angle outliers ?

*There are 614 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	112.60	136.32	1
CA-CB-CG	112.60	93.15	1
C-N-CA	121.70	154.98	1
C-N-CA	121.70	154.05	1
C-N-CA	121.70	153.70	1
CA-CB-CG	113.80	96.09	1
C-N-CA	121.70	153.31	1
N-CA-C	111.00	64.94	1
C-CA-CB	110.10	137.83	1
CA-CB-CG	113.80	99.23	1
CA-C-O	120.80	96.75	1
C-N-CA	121.70	147.02	1
C-N-CA	121.70	146.60	1
C-N-CA	121.70	145.74	1
N-CA-C	111.00	74.59	1
C-CA-CB	110.10	86.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	133.91	1
C-CA-CB	110.10	86.54	1
C-N-CA	121.70	99.61	1
CA-CB-CG	113.80	101.87	1
N-CA-C	112.10	141.57	1
N-CA-C	111.00	78.13	1
CA-C-N	116.20	139.50	1
CA-CB-CG	112.60	123.47	1
C-N-CA	121.70	141.00	1
C-N-CA	121.70	102.48	1
CA-CB-CG	112.60	101.99	1
C-N-CA	121.70	102.64	1
N-CA-CB	111.50	93.52	1
C-N-CA	121.70	140.61	1
CA-CB-CG2	110.50	92.77	1
N-CA-CB	110.50	128.20	1
N-CA-C	111.00	140.08	1
C-CA-CB	110.10	90.37	1
C-CA-CB	111.60	132.36	1
N-CA-C	111.00	82.06	1
CA-C-N	116.90	132.24	1
C-N-CA	121.70	140.10	1
O-C-N	123.00	139.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	139.92	1
C-N-CA	121.70	139.90	1
C-CA-CB	110.10	90.89	1
CA-CB-CG	112.60	122.67	1
C-N-CA	121.70	139.71	1
CA-CB-CG	113.80	103.80	1
CA-CB-CG	113.80	103.90	1
CA-CB-CG	113.80	103.94	1
CA-C-N	116.20	135.90	1
N-CA-C	111.00	138.24	1
CA-CB-CG	112.60	102.87	1
C-N-CA	121.70	139.07	1
N-CA-C	111.00	84.14	1
C-N-CA	121.70	138.85	1
C-N-CA	121.70	138.83	1
CA-C-N	116.20	135.14	1
CA-CB-CG	113.80	104.39	1
N-CA-C	111.00	137.28	1
CA-CB-CG	113.80	104.47	1
CA-N-CD	112.00	99.08	1
C-N-CA	121.70	138.29	1
N-CA-CB	110.50	126.10	1
CA-C-N	116.90	103.19	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	126.01	1
O-C-N	123.00	108.57	1
C-N-CA	121.70	105.54	1
N-CA-C	111.00	85.89	1
C-N-CA	121.70	137.78	1
C-N-CA	121.70	137.57	1
C-N-CA	121.70	137.48	1
CA-CB-CG2	110.40	95.52	1
CA-C-O	120.80	105.94	1
C-N-CA	121.70	137.26	1
C-CA-CB	110.10	93.71	1
C-N-CA	121.70	106.24	1
N-CA-C	111.00	87.03	1
N-CA-C	111.00	87.21	1
CA-CB-CG2	110.40	124.82	1
N-CA-C	111.00	87.36	1
N-CA-CB	110.40	97.75	1
N-CA-C	111.00	87.54	1
CA-CB-CG	113.80	105.43	1
C-N-CA	121.70	106.79	1
C-N-CA	121.70	136.55	1
N-CA-CB	111.50	97.63	1
N-CA-C	111.00	88.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	132.43	1
CA-CB-CG2	110.40	124.11	1
CA-CB-CG1	110.40	96.75	1
N-CA-C	111.00	133.44	1
CA-C-N	116.20	132.19	1
CA-CB-CG1	110.40	96.83	1
C-CA-CB	110.10	94.95	1
CA-C-N	116.20	132.07	1
C-N-CA	121.70	135.95	1
C-CA-CB	110.10	95.18	1
C-CA-CB	111.40	96.52	1
C-N-CA	121.70	107.63	1
C-N-CA	121.70	107.64	1
C-N-CA	121.70	107.73	1
C-N-CA	121.70	135.66	1
CA-CB-CG	114.10	98.61	1
C-CA-CB	111.40	96.68	1
CA-C-N	116.20	131.67	1
C-N-CA	121.70	107.81	1
N-CA-CB	110.50	97.40	1
CA-C-N	116.20	131.58	1
C-N-CA	121.70	135.50	1
N-CA-CB	110.50	97.48	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	105.01	1
C-N-CA	121.70	108.05	1
C-CA-CB	110.10	95.73	1
C-N-CA	121.70	108.10	1
C-N-CA	121.70	135.23	1
CA-CB-CG1	110.40	97.63	1
CA-CB-CG	113.90	100.43	1
CA-CB-CG	113.80	106.32	1
CA-CB-CG	113.80	106.33	1
C-CA-CB	110.10	124.28	1
CA-C-N	116.90	128.08	1
CA-CB-CG	112.60	105.16	1
C-N-CA	121.70	108.34	1
C-N-CA	121.70	108.35	1
N-CA-CB	111.50	98.91	1
N-CA-CB	110.50	123.07	1
CA-C-N	116.20	130.81	1
N-CA-C	111.00	131.43	1
C-CA-CB	110.10	123.94	1
C-N-CA	121.70	134.81	2
N-CA-C	113.30	92.18	1
C-CA-CB	110.10	96.37	1
N-CA-CB	110.50	98.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	131.08	1
C-N-CA	121.70	108.79	1
N-CA-C	112.10	130.00	1
N-CA-C	111.00	90.96	1
N-CA-CB	111.50	123.62	1
N-CA-C	111.00	91.13	1
O-C-N	123.00	111.65	1
CA-CB-CG	114.10	99.92	1
C-CA-CB	110.10	123.57	1
CA-CB-CG	113.80	106.73	1
CA-CB-CG	114.10	99.96	1
C-N-CA	121.70	108.98	1
N-CA-C	111.00	91.25	1
N-CA-CB	110.50	122.46	1
CA-CB-CG	113.80	106.82	1
CB-CG-CD	112.60	100.74	1
C-N-CA	121.70	134.23	1
CA-CB-CG	112.60	105.69	1
C-N-CA	121.70	109.28	1
N-CA-C	111.00	91.77	1
C-CA-CB	111.60	97.86	1
CA-C-O	120.80	109.14	1
N-CA-C	111.00	91.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	109.20	1
N-CA-C	111.00	91.90	1
CA-CB-CG	113.80	106.98	1
N-CA-C	111.00	130.10	1
C-N-CA	121.70	109.42	1
CA-CB-CG1	110.40	121.97	1
CA-CB-CG	113.80	107.00	1
C-N-CA	121.70	109.50	1
N-CA-C	111.00	92.04	1
CG1-CB-CG2	110.80	125.66	1
N-CA-CB	110.50	121.97	1
CA-C-O	120.80	109.33	1
N-CA-C	111.00	92.11	1
N-CA-C	111.00	129.86	1
C-N-CA	121.70	109.61	1
C-N-CA	121.70	109.68	1
CB-CG-CD	112.60	101.30	1
CA-CB-CG	112.60	119.23	1
O-C-N	123.00	112.39	1
N-CA-C	112.10	95.57	1
CA-CB-CG	113.60	101.07	1
CA-CB-CG	112.60	106.01	1
C-N-CA	121.70	109.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	112.52	1
CA-CB-CG	114.10	101.03	1
CA-CB-CG	113.80	107.26	1
O-C-N	123.00	133.45	1
CA-CB-CG	112.60	106.10	1
N-CA-C	111.00	92.81	1
C-N-CA	121.70	133.39	1
C-CA-CB	110.10	122.43	1
N-CA-CB	110.50	121.49	1
C-N-CA	121.70	110.06	1
O-C-N	123.00	112.68	1
N-CA-C	111.00	128.99	1
C-N-CA	121.70	110.14	1
C-N-CA	121.70	133.19	1
C-CA-CB	110.10	122.17	2
N-CA-C	112.10	96.22	1
CA-CB-CG	112.60	106.26	1
C-CA-CB	110.10	98.06	1
C-N-CA	121.70	110.32	1
C-N-CA	121.70	133.06	1
C-N-CA	121.70	110.37	1
N-CA-CB	110.50	121.15	1
C-N-CA	121.70	132.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	110.44	1
C-N-CA	121.70	132.96	1
C-CA-CB	110.10	121.97	1
N-CA-C	111.00	93.57	1
CA-C-N	116.90	126.23	1
C-N-CA	121.70	110.50	1
C-N-CA	121.70	110.52	1
C-N-CA	121.70	132.81	1
O-C-N	123.00	132.85	1
CA-CB-CG	113.80	107.66	1
C-CA-CB	110.10	121.69	1
CA-CB-CG	114.10	101.91	1
N-CA-C	113.30	95.65	1
C-N-CA	121.70	110.75	1
CA-CB-CG	113.90	102.97	1
N-CA-C	111.00	94.02	1
CA-CB-CG1	110.40	100.10	1
C-CA-CB	109.10	122.43	1
N-CA-C	111.00	127.94	1
C-CA-CB	110.50	119.57	1
CA-CB-CG	113.80	107.76	2
CA-CB-CG	113.90	103.05	1
N-CA-C	111.00	127.87	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	107.80	1
C-N-CA	121.70	110.91	1
C-N-CA	121.70	132.41	1
CA-CB-CG	113.90	103.20	1
C-N-CA	121.70	111.07	1
N-CA-C	111.00	94.47	1
N-CA-CB	110.50	120.50	1
C-CA-CB	111.60	99.84	1
CA-CB-OG1	109.60	100.79	1
C-CA-CB	111.60	99.86	1
CA-C-O	120.80	110.87	1
CA-CB-CG2	110.50	100.57	1
O-C-N	123.00	132.34	1
CA-CB-CG	113.80	107.97	1
N-CA-C	111.00	94.69	1
CA-CB-CG	112.60	106.78	1
N-CA-CB	111.50	101.61	1
N-CA-C	111.00	94.71	1
N-CA-CB	111.50	121.38	1
CA-CB-CG	113.80	108.00	1
CA-C-N	116.90	125.57	1
C-CA-CB	110.10	121.02	1
C-N-CA	121.70	111.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	125.51	1
C-N-CA	121.70	111.41	2
C-N-CA	121.70	131.91	1
O-C-N	123.00	132.05	1
CA-C-N	116.90	108.43	1
CA-C-O	120.80	111.20	1
C-N-CA	121.70	111.55	1
CA-C-N	116.20	127.45	1
C-N-CA	121.70	111.63	1
N-CA-CB	110.50	101.02	1
C-N-CA	121.70	131.73	1
CA-C-O	120.80	111.38	1
C-N-CA	121.70	111.73	1
CA-CB-CG	113.80	108.28	1
CA-CB-CG	113.90	103.98	1
N-CA-C	111.00	126.37	1
C-CA-CB	110.10	99.68	1
CA-CB-CG	113.90	104.04	1
N-CA-C	111.00	95.66	1
N-CA-CB	110.50	119.79	1
C-N-CA	121.70	111.87	2
C-CA-CB	109.10	97.08	1
C-N-CA	121.70	131.48	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	107.17	2
N-CA-C	111.00	126.17	1
C-N-CA	121.70	111.98	1
C-CA-CB	110.10	99.85	1
C-N-CA	122.60	95.67	1
N-CA-CB	103.00	108.92	1
C-CA-CB	110.10	120.32	1
O-C-N	123.00	131.60	1
C-CA-CB	110.10	99.90	1
N-CA-CB	110.50	101.38	1
N-CA-CB	110.50	119.60	1
N-CA-C	111.00	96.03	1
CA-CB-CG	112.60	107.26	1
CA-C-N	116.90	108.91	1
C-N-CA	121.70	112.12	1
CA-CB-CG2	110.40	101.35	1
N-CA-CB	110.50	119.53	1
C-N-CA	121.70	131.26	1
CA-C-O	120.80	111.79	1
N-CA-C	113.30	97.93	1
N-CA-CB	111.50	120.50	1
C-CA-CB	110.10	100.05	1
C-CA-CB	110.10	100.10	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	119.35	1
C-N-CA	121.70	131.17	1
N-CA-CB	110.50	119.44	1
N-CA-C	111.00	96.31	1
CA-CB-CG	112.60	107.36	1
C-CA-CB	110.10	120.04	1
CA-CB-CG	113.90	104.50	1
N-CA-C	112.10	125.16	1
CA-C-O	120.80	111.92	1
CA-CB-CG	112.60	107.40	1
CA-CB-CG	112.60	107.41	1
C-CA-CB	110.10	119.96	1
C-N-CA	121.70	112.36	1
N-CA-CB	110.50	119.32	1
N-CA-C	111.00	125.52	1
O-C-N	123.00	114.71	1
N-CA-CB	110.50	119.31	1
C-N-CA	121.70	112.38	1
C-CA-CB	111.40	101.57	1
CA-CB-CG	113.90	104.59	1
N-CA-C	111.00	96.53	1
CA-CB-CG	112.60	107.43	1
C-N-CA	121.70	112.40	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	96.54	1
CA-C-N	116.20	105.90	1
N-CA-CB	110.50	119.25	1
CA-CB-CG	113.80	108.66	1
C-CA-CB	110.10	119.86	1
CA-C-N	116.20	126.46	1
N-CA-CB	110.50	119.21	1
CA-CB-CG	113.80	108.67	1
C-CA-CB	110.10	100.36	1
CA-CB-CG	112.60	107.48	1
C-N-CA	121.70	130.89	2
C-N-CA	121.70	112.54	1
C-CA-CB	110.10	100.43	1
CA-CB-CG	112.60	107.52	1
CA-C-N	116.20	106.03	1
N-CA-CB	103.00	108.57	1
C-N-CA	121.70	112.59	1
N-CA-C	111.00	96.84	1
N-CA-C	111.00	125.10	1
CA-C-N	116.20	126.26	1
N-CA-CB	110.50	119.05	1
N-CA-C	112.10	99.54	1
O-C-N	123.00	114.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	114.97	1
CA-C-N	116.20	126.23	1
N-CA-CB	111.50	120.02	1
C-CA-CB	109.10	120.11	1
CA-CB-CG	112.60	107.59	1
CA-C-N	116.90	109.40	1
C-N-CA	121.70	130.70	1
C-N-CA	121.70	130.65	1
CA-CB-CG1	110.40	118.83	1
C-N-CD	125.00	104.68	1
C-N-CA	121.70	112.79	1
CA-C-N	116.90	109.48	1
N-CA-C	112.10	99.73	1
N-CA-C	113.30	98.98	1
O-C-N	123.00	130.88	1
CA-CB-CG	112.60	107.68	2
N-CA-C	111.00	124.78	1
N-CA-C	111.00	97.23	1
N-CA-CB	103.00	108.40	1
CA-C-N	116.20	126.02	1
CA-C-N	116.90	124.27	1
CA-CB-CG	112.60	107.71	2
C-CA-CB	109.10	119.86	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	112.90	1
N-CA-C	111.00	124.67	1
C-N-CA	121.70	130.47	1
N-CA-CB	111.50	119.77	1
C-N-CA	121.70	130.45	1
CA-CB-CG	112.60	107.74	1
C-N-CA	121.70	130.44	1
C-CA-CB	110.10	100.88	1
CA-CB-CG	113.80	108.95	1
CA-CB-CG	112.60	107.75	1
N-CA-CB	110.50	102.28	1
CA-CB-CG	112.60	107.77	1
N-CA-C	111.00	97.48	1
O-C-N	123.00	115.29	1
C-CA-CB	111.60	101.96	1
C-N-CA	121.70	130.37	1
C-N-CA	121.70	113.03	1
CB-CG-CD	112.60	120.78	1
CA-CB-CG	114.10	104.48	1
O-C-N	123.00	130.70	1
C-N-CA	121.70	113.04	1
C-N-CA	121.70	113.06	1
CA-C-N	116.90	124.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	112.67	1
CA-C-O	120.80	112.68	1
N-CA-CB	110.50	118.62	1
C-CA-CB	110.10	101.03	1
N-CA-CB	110.50	118.60	1
CA-CB-CG	113.60	104.55	1
C-N-CA	121.70	113.16	1
CA-CB-CG	112.60	107.85	1
O-C-N	123.00	115.41	1
CD2-NE2-CE1	109.00	104.27	1
CA-CB-CG	113.80	109.08	1
O-C-N	123.00	115.44	1
CA-CB-CG	112.60	107.88	1
CA-CB-CG	113.90	105.42	1
CA-CB-CG	113.80	109.09	2
CA-CB-CG	112.60	107.89	1
N-CA-CB	110.50	118.49	1
C-N-CA	121.70	130.15	1
CA-CB-CG	112.60	107.91	1
N-CA-C	111.00	97.88	1
O-C-N	123.00	115.51	1
C-N-CA	121.70	130.12	1
CD-NE-CZ	124.40	117.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	124.09	1
CA-CB-CG	112.60	107.93	1
CA-C-N	116.20	125.50	1
C-CA-CB	110.10	101.26	1
CA-C-N	116.90	109.92	1
CB-CG-CD	112.60	104.70	1
CA-CB-CG	112.60	107.96	1
N-CA-C	111.00	98.03	1
C-CA-CB	111.60	102.34	1
N-CA-C	112.10	100.53	1
C-N-CA	121.70	113.38	1
C-N-CA	121.70	113.41	1
CA-CB-CG	113.80	109.20	1
C-N-CA	121.70	129.98	1
N-CA-CB	110.50	118.31	1
CA-CB-CG	112.60	117.19	1
CA-C-N	116.20	125.37	1
C-N-CA	121.70	129.95	1
O-C-N	123.00	115.67	1
CA-C-N	116.20	107.05	1
CB-CG-CD	111.30	121.80	1
N-CA-CB	110.50	118.26	1
C-N-CA	121.70	113.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	130.30	1
C-CA-CB	110.10	101.44	1
CA-CB-CG	113.80	109.25	2
C-CA-CB	110.50	103.67	1
CB-CG-CD	112.60	104.87	1
CA-CB-CG	112.60	108.06	1
C-N-CA	121.70	113.52	1
N-CA-C	111.00	98.29	1
CD2-NE2-CE1	109.00	104.46	1
C-CA-CB	110.10	101.49	1
C-N-CA	121.70	113.54	1
N-CA-C	111.00	123.68	1
CA-C-N	116.90	123.69	1
C-CA-CB	110.10	118.70	1
N-CA-C	111.00	123.67	1
N-CA-CB	110.50	118.19	1
CA-CB-CG	113.80	118.31	1
N-CA-C	113.30	100.23	1
N-CA-CB	111.50	119.16	1
CD2-NE2-CE1	109.00	104.50	1
C-N-CA	121.70	129.80	1
N-CA-C	111.00	98.41	1
CA-CB-CG	112.60	108.11	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	125.17	1
N-CA-C	111.00	98.45	1
N-CA-CB	110.50	118.12	1
CG1-CB-CG2	110.80	120.66	1
C-CA-CB	111.40	119.92	1
CA-C-N	116.20	125.16	1
C-N-CA	121.70	129.76	1
C-N-CA	121.70	113.64	1
CA-C-N	116.20	125.14	1
N-CA-CB	111.50	103.90	1
CD2-NE2-CE1	109.00	104.53	1
N-CA-C	113.30	100.35	1
CA-CB-CG	112.60	108.13	1
CA-CB-CG	112.60	108.14	1
CD2-NE2-CE1	109.00	104.54	2
N-CA-CB	110.50	102.93	1
C-N-CA	121.70	129.72	1
CD2-NE2-CE1	109.00	104.55	2
N-CA-C	111.00	123.46	1
CD2-NE2-CE1	109.00	104.56	2
N-CA-C	111.00	98.57	1
CA-C-O	119.00	105.69	1
CA-CB-CG	112.60	108.17	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	104.58	2
CG-SD-CE	100.90	91.18	1
CA-CB-CG	112.60	108.18	1
CA-C-N	116.20	125.02	1
CD2-NE2-CE1	109.00	104.59	2
C-CA-CB	111.40	103.04	1
CA-C-O	120.80	113.32	1
N-CA-CB	110.50	117.95	1
CA-C-N	116.90	123.47	1
C-N-CA	121.70	113.82	2
N-CA-CB	110.40	116.96	1
N-CA-CB	110.50	117.93	2
C-N-CA	121.70	113.83	1
CD2-NE2-CE1	109.00	104.63	1
C-N-CA	121.70	113.84	1
CA-C-N	116.20	124.91	1
CA-C-N	116.90	110.39	1
CA-C-N	116.90	123.41	1
CA-CB-CG	112.60	108.26	1
CG-SD-CE	100.90	91.36	1
CA-CB-CG	112.60	108.28	1
N-CA-C	112.10	122.90	1
N-CA-C	113.30	125.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.84	1
CD2-NE2-CE1	109.00	104.68	1
C-N-CA	121.70	113.94	2
N-CA-C	111.00	123.06	1
N-CA-CB	110.50	117.82	1
CA-CB-CG	112.60	108.30	1
CA-CB-CG	113.80	118.10	1
CB-CG-CD	112.60	105.29	1
CA-CB-CG	112.60	108.31	2
C-N-CA	121.70	113.98	1
C-CA-CB	110.10	101.96	1
CA-CB-CG1	110.40	117.68	1
CA-C-N	116.20	124.77	1
CA-CB-CG	113.80	109.52	1
CB-CG-CD	112.60	105.34	1
C-N-CA	121.70	114.01	2
O-C-N	123.00	129.82	1
CD-NE-CZ	124.40	118.44	1
C-N-CA	121.70	114.04	1
C-N-CA	121.70	114.05	1
C-CA-CB	110.10	102.03	1
CA-CB-CG	112.60	108.36	1
C-N-CA	121.70	114.07	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	114.08	1
C-N-CA	121.70	129.32	1
CA-C-O	120.80	113.61	1
N-CA-C	111.00	122.82	1
CD-NE-CZ	124.40	118.49	1
N-CA-C	111.00	122.80	1
C-N-CA	121.70	114.12	1
N-CA-CB	103.00	107.62	1
CA-CB-CG	112.60	108.41	1
CG1-CB-CG2	110.80	120.01	1
C-N-CA	121.70	114.18	1
N-CA-C	111.00	122.69	1
CB-CG-CD1	120.80	127.06	1
CA-CB-CG2	110.50	103.41	1
N-CA-CB	110.50	103.41	1
CA-CB-CG	112.60	108.44	1
N-CA-CB	111.50	118.55	1
N-CA-C	111.00	99.40	1
N-CA-CB	110.50	117.54	1
N-CA-C	111.00	99.41	1
CA-CB-CG	113.90	106.45	1
N-CA-CB	110.50	117.53	1
C-N-CA	121.70	114.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	111.30	120.79	1
C-N-CA	121.70	114.28	1
CA-CB-CG	112.60	108.48	2
CA-C-O	120.80	113.79	1
N-CA-CB	111.50	118.50	1
N-CA-C	111.00	99.51	1
CA-CB-CG2	110.50	103.53	1
C-N-CA	121.70	114.32	1
CA-CB-CG	114.10	105.91	1
CA-C-O	120.80	127.76	1
C-N-CA	121.70	129.06	1
N-CA-CB	110.50	117.45	1
N-CA-C	111.00	99.57	1
N-CA-CB	103.00	107.49	1
C-CA-CB	110.10	102.35	1
N-CA-CB	110.50	117.43	1
C-CA-CB	111.40	119.14	1
O-C-N	123.00	116.49	1
CA-CB-CG	112.60	108.53	1
C-N-CA	121.70	129.02	1
C-N-CA	121.70	114.38	1
CA-CB-CG	113.90	106.58	1
CA-CB-CG	112.60	108.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	122.22	1
C-CA-CB	109.10	118.03	1
C-N-CA	121.70	129.01	1
O-C-N	123.00	116.52	1
CA-CB-CG	112.60	108.55	1
CA-C-N	116.20	124.27	1
N-CA-C	111.00	99.71	1
CA-CB-CG	112.60	108.57	1
N-CA-CB	110.50	103.66	1
CA-CB-CG2	110.40	117.24	1
C-N-CA	121.70	114.46	1
N-CA-C	111.00	99.74	1
C-N-CA	121.70	114.47	1
C-N-CA	121.70	128.93	1
O-C-N	123.00	116.57	1
CA-CB-CG	113.80	109.79	1
CA-CB-CG	112.60	108.59	2
C-N-CA	121.70	128.92	1
N-CA-CB	110.50	117.31	1
C-CA-CB	110.50	104.50	1
CA-C-N	116.20	124.20	1
N-CA-C	111.00	99.80	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	0.00	0

All 0 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	Analysed	Favored	Allowed	Outliers
1	892	755	79	58

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	812	676	71	65

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	22	OMET
1	A	24	OLYS
1	A	27	OHIS
1	A	41	OARG
1	A	60	OLEU
1	A	79	OGLU
1	A	96	OLYS
1	A	117	OLYS
1	A	132	OGLN

Model ID	Chain	Residue ID	Residue type
1	A	134	OLYS
1	A	143	OLEU
1	A	191	OTRP
1	A	194	OASN
1	A	203	OILE
1	A	251	OLYS
1	A	260	0GLU
1	A	294	OLEU
1	A	300	0GLU
1	A	316	0PHE
1	A	320	OLYS
1	A	328	OTRP
1	A	330	OILE
1	A	332	OASN
1	A	333	OVAL
1	A	334	OLEU
1	A	338	OILE
1	A	352	0TYR
1	A	354	0ARG
1	A	358	OLYS
1	A	379	OVAL
1	B	27	0HIS
1	B	48	0ARG

Model ID	Chain	Residue ID	Residue type
1	B	50	0ARG
1	B	60	0LEU
1	B	72	0ASN
1	B	96	0LYS
1	B	117	0LYS
1	B	125	0MET
1	B	179	0TYR
1	B	185	0ARG
1	B	195	0LYS
1	B	255	0THR
1	B	309	0ASN
1	B	320	0LYS
1	B	325	0GLU
1	B	328	0TRP
1	B	334	0LEU
1	B	341	0LYS
1	B	342	0LYS
1	B	352	0TYR
1	B	379	0VAL
1	B	395	0LYS
1	C	3	0GLU
1	C	16	0THR
1	C	23	0LYS



Model ID	Chain	Residue ID	Residue type
1	C	32	0GLN
1	C	35	0GLN
1	C	37	0LYS
1	C	39	0LYS
1	C	42	0LYS
1	D	4	0ASN
1	D	22	0ARG
1	D	23	0LYS
1	D	37	0LYS
1	D	45	0VAL

### Fit of model to data used for modeling ?

#### Crosslinking-MS

Validation for this section is under development.

### Fit of model to data used for validation ?

Validation for this section is under development.

#### *Acknowledgements*

*Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.*

*Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in*

*implementing SAS validation methods.*

*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*