

# Integrative Structure Validation Report

July 22, 2024 - 04:09 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	9A0I
PDB-Dev ID	PDBDEV_00000054
Structure Title	Structural model of UDP-glucose:glycoprotein glucosyl-transferase bound to Fab
Structure Authors	Modenutti CP; Blanco Capurro JI; Ibba R; Alonzi DS; Song MN; Vasiljevic S; Kumar A; Chandran AV; Tax G; Marti L; Hill JC; Lia A; Hensen M; Waksman T; Rushton J; Rubichi S; Santino A; Marti MA; Zitzmann N; Roversi P

*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)*

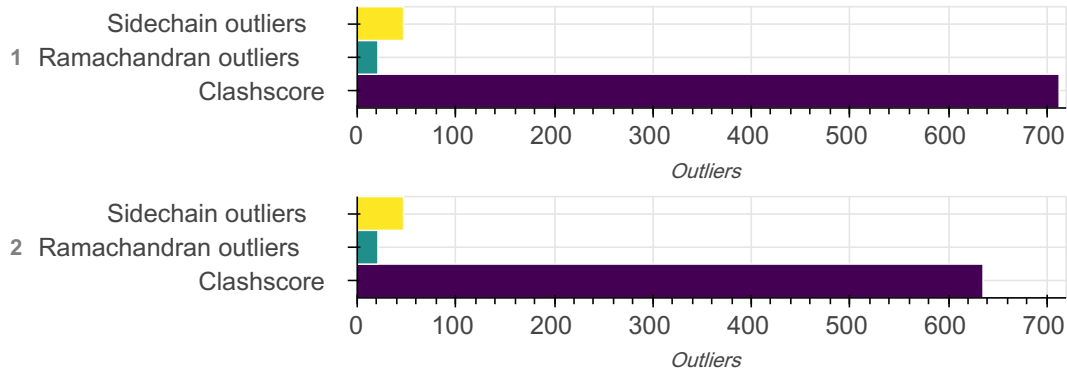
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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 2 unique models, with 3 subunits in each model. A total of 7 datasets or restraints were used to build this entry. Each model is represented by 16 rigid bodies and 0 flexible or non-rigid units.*

## Entry composition ?

*There are 2 unique types of models in this entry. These models are titled None/Model fit into the original hand of the EM map, None/Model fit into the inverse hand of the EM map respectively.*

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	TdUGGT	A	A	1368
1	2	2	Fab Heavy Chain	B	L	214
1	3	3	Fab Light Chain	C	H	214
2	1	1	TdUGGT	A	A	1368
2	2	2	Fab Heavy Chain	B	L	214
2	3	3	Fab Light Chain	C	H	214

## Datasets used for modeling ?

There are 7 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	3DEM volume	EMDB	EMD-30386
2	Other	File	10.1038/s41598-017-12283-w
3	Experimental model	PDB	5Y7O
4	Experimental model	PDB	5MU1
5	Experimental model	PDB	5H18
6	Experimental model	PDB	1FGN
None	Other	Not available	Not available

## Representation ?

This entry has only one representation and includes 16 rigid bodies and 0 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-129, 130-137, 138-222, 223-342, 343-354, 355-623, 624-633, 634-677, 678-681, 682-695, 696-699, 700-977, 978-1091, 1092-1368	-
B	1-214	-
C	1-214	-

## 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
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Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	Fitting the TdUGGT and Fab models in the negative stain EM map	None	None	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	<a href="#">Coot</a>	Not available	model building	<a href="https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/">https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/</a>
2	<a href="#">Modeller</a>	Not available	model building	<a href="https://salilab.org/modeller/">https://salilab.org/modeller/</a>
3	<a href="#">Chimera</a>	Not available	visualization	<a href="https://www.cgl.ucsf.edu/chimera/">https://www.cgl.ucsf.edu/chimera/</a>

## Data quality

### 3DEM volume

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 455 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
C-N-CA	121.70	82.62	1
C-N-CA	121.70	82.65	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CA-CB-CA-CB-CG	113.80	102.67	1
CA-CB-CG	113.80	102.72	1
C-N-CA-CB-CA-CB-C-N-CA-CB-CA-CB-CA-CB-CG	112.60	102.58	1
CA-CB-CG	112.60	102.58	1
CA-CB-CG	113.80	103.85	1
CA-CB-CG	113.80	103.88	1
C-N-CA	121.70	104.03	1
C-N-CA	121.70	104.16	1
CA-CB-CA-CB-CA-CB-CG	113.80	104.94	1
CA-CB-CG	113.80	104.96	1
C-N-CA	121.70	137.45	1
C-N-CA	121.70	137.43	1
N-CA-N-CA-CA-C-CA-C-C-N-CA	121.70	107.15	1
C-N-CA	121.70	107.15	1
N-CA-C	110.74	134.83	1
N-CA-C	110.74	134.80	1
CA-CB-CG	113.80	106.04	1
CA-CB-CG	113.80	106.06	1
C-N-C-N-C-N-CA	121.70	107.98	1
C-N-CA	121.70	107.99	1
CA-CB-CG	113.80	106.21	2
C-CA-CB	110.50	99.18	1
C-CA-CB	110.50	99.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	106.44	1
CA-CB-CG	113.80	106.46	1
CA-CB-CG	113.90	100.70	2
CA-CB-CG	113.80	106.51	1
CA-CB-CG	113.80	106.52	1
C-N-CA	121.70	134.31	1
C-N-CA	121.70	134.30	1
CA-CB-CG	113.80	106.81	2
C-N-CA	121.70	134.26	1
CA-CB-CG	113.80	106.82	1
C-N-CA	121.70	134.24	1
CA-CB-CA-CB-CG	113.80	106.85	1
CA-CB-CG	112.60	105.66	1
CA-CB-CA-CB-CG	112.60	105.71	1
C-N-CA	121.70	109.30	1
C-N-CA	121.70	109.36	1
CA-CB-CA-CB-CA-CB-CA-CB-CA-CB-CG	112.60	105.80	1
CA-CB-CG	112.60	105.80	1
CA-CB-CA-CB-CA-CB-CA-CB-CG	113.80	107.17	1
CA-CB-CA-CB-CG	113.80	107.19	1
CA-CB-CG	113.90	102.10	1
CA-CB-CG	113.90	102.11	1
CA-CB-CA-CB-CA-CB-CG	113.80	107.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	107.30	1
C-CA-C-CA-CA-CB-CG	113.80	107.37	1
CA-CB-CG	113.80	107.39	1
N-CA-C	110.74	91.69	1
N-CA-C	110.74	91.72	1
C-N-CA	121.70	133.08	1
C-N-CA	121.70	133.02	1
C-N-CA	121.70	132.98	1
C-N-CA	121.70	132.97	1
CA-CB-CG	113.90	102.64	1
CA-CB-CA-CB-CG	113.90	102.68	1
CA-CB-CG	113.80	107.57	1
CA-CB-CG	113.80	107.58	1
CA-CB-CA-CB-CG	113.80	107.61	1
CA-CB-CG	113.80	107.65	1
CB-CG-CD	112.60	102.18	1
CA-CB-CG	113.80	107.69	1
CA-CB-CA-CB-CG	113.80	107.70	1
N-CA-C	110.74	92.44	1
N-CA-C	110.74	92.46	1
CB-CG-CD	112.60	102.26	1
CA-CB-N-CA-C	111.00	93.98	1
N-CA-C	111.00	93.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	107.75	2
N-CA-CB	110.40	119.42	1
N-CA-CB	110.40	119.41	1
CA-C-CA-CB-CA-CB-C-N-CA	121.70	110.94	1
C-N-CA	121.70	110.95	1
CA-C-CA-CB-CG	113.80	107.85	1
CA-CB-CG	112.60	106.68	2
CA-CB-CG	113.80	107.90	1
C-N-CA	121.70	132.30	2
CA-CB-CG	112.60	106.74	1
CA-CB-CG	112.60	106.75	2
CA-CB-CG	112.60	106.76	1
CA-CB-CG	112.60	106.77	1
CA-CB-CG	112.60	106.78	1
CA-CB-CA-CB-CG	112.60	106.79	1
CA-CB-N-CA-C	113.30	96.45	1
N-CA-C	113.30	96.45	1
CA-CB-CG	112.60	106.80	2
N-CA-CB	110.50	100.64	2
CA-C-N	116.90	125.59	1
CA-C-N	116.90	125.55	1
N-CA-CB	110.50	120.30	1
CA-CB-CG	112.60	106.84	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	120.27	1
C-N-CA	121.70	132.02	1
C-N-CA	121.70	132.00	1
CA-CB-CG	113.80	108.10	1
CA-CB-CG	113.80	108.11	1
O-C-N	123.00	113.92	1
O-C-N	123.00	113.95	1
C-CA-CB	109.10	121.55	1
N-CA-C	111.00	126.83	1
CA-CB-N-CA-C	111.00	126.75	1
C-N-C-CA-CB	109.10	121.46	1
CA-CB-CG	112.60	106.98	2
C-N-CA	121.70	131.78	1
CA-CB-CG	112.60	107.00	1
C-CA-CB	110.10	120.74	1
C-N-C-N-C-CA-CB	110.10	120.70	1
CA-CB-C-N-CA-CB-CG	112.60	107.06	1
N-CA-C	111.00	95.52	1
N-CA-C	111.00	95.53	1
C-N-CA	121.70	131.64	2
C-N-CA	121.70	131.61	1
CA-CB-CG	112.60	107.12	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	107.13	1
C-CA-CB	111.40	101.02	1
CA-CB-CG	113.80	108.35	2
CA-CB-CG	112.60	107.16	1
C-CA-CB	111.40	101.08	1
CA-CB-N-CA-CB	110.50	119.72	1
CA-CB-CG	112.60	107.18	1
CA-CB-CA-CB-C-N-CA	121.70	131.44	1
N-CA-CB	110.50	119.69	1
C-N-CA	121.70	112.00	1
CA-CB-CG	113.80	108.42	2
CA-CB-CG	112.60	107.23	1
CA-CB-N-CA-CB	110.50	119.60	1
N-CA-CB	110.50	119.60	1
C-N-CA	121.70	112.06	1
C-N-CA	121.70	131.34	1
CA-CB-CA-CB-CG	112.60	107.26	1
CA-CB-CA-CB-CA-CB-CG	112.60	107.29	1
CA-CB-C-N-CA	121.70	131.20	1
C-N-CA	121.70	112.21	1
C-N-C-N-CA	121.70	131.17	1
CA-CB-CG	112.60	107.34	1
C-N-CA-CB-C-CA-C-CA-CA-CB-CA-CB-CG	113.90	104.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	112.29	1
C-CA-CB	110.10	120.04	1
CA-CB-CA-CB-CG	113.90	104.51	1
C-CA-CB	110.10	120.01	1
CA-CB-CA-C-C-N-CA	121.70	131.07	1
C-N-CA	121.70	131.07	2
CA-CB-CG	112.60	107.40	2
CA-CB-CA-CB-CG	112.60	107.41	1
CA-C-C-N-CA	121.70	131.02	1
CA-CB-CA-CB-CA-CB-CA-CB-CG	112.60	107.44	1
CA-CB-CG	112.60	107.46	2
CA-CB-CB-CG-CD	112.60	103.90	1
CA-CB-CG	112.60	107.48	1
CA-CB-CG	112.60	107.49	1
CA-CB-C-N-CA-CB-C-N-CA-CB-CG	112.60	107.51	1
CA-CB-CG	112.60	107.52	2
C-N-CB-CG-CD	112.60	103.97	1
CA-CB-N-CA-CB	110.50	101.88	1
CA-CB-C-N-N-CA-C	110.74	125.92	1
N-CA-C	110.74	125.89	1
CA-CB-C-N-CA-CB-CG	112.60	107.57	1
N-CA-CB	110.50	101.95	1
N-CA-CB	110.50	101.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA-CB-CG	112.60	107.60	1
CA-CB-CG	112.60	107.60	1
N-CA-CB	110.50	102.00	1
N-CA-C	110.74	125.74	1
CA-CB-CA-CB-N-CA-C	110.74	125.71	1
CA-C-N	116.90	124.38	1
CA-C-N	116.90	124.37	1
CA-CB-CG	112.60	107.62	1
CA-CB-CG	112.60	107.63	1
N-CA-CB	110.50	102.06	1
C-N-CA-CB-CG	112.60	107.64	1
C-N-CA-CB-CG	112.60	107.65	1
C-CA-CB	110.10	119.51	1
CA-CB-CG	112.60	107.65	1
CA-CB-CG	112.60	107.66	1
C-CA-CB	110.10	119.48	1
N-CA-CB	110.50	102.11	1
C-CA-CA-CB-CG	112.60	107.67	1
CA-CB-CG	112.60	107.67	2
C-CA-CA-CB-CG	112.60	107.69	1
N-CA-CB	110.50	102.16	1
N-CA-CB	110.50	102.17	2
CA-CB-CG	112.60	107.70	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.90	105.08	1
CA-CB-CA-CB-CG	112.60	107.71	1
C-N-CA	121.70	130.50	2
N-CA-CB	110.50	102.20	1
CA-CB-CG	113.90	105.11	1
CA-CB-C-CA-CB	110.10	100.85	1
C-CA-CB	110.10	100.85	1
C-CA-N-CA-CB	110.50	102.23	1
C-N-CA	121.70	130.45	1
CA-CB-C-CA-C-N-CA	121.70	130.43	1
N-CA-CB	110.50	102.27	2
N-CA-C	110.74	125.26	1
N-CA-C	110.74	125.25	1
CA-CB-CA-CB-CG	112.60	107.78	1
CA-CB-CG	112.60	107.78	1
N-CA-CB	110.50	102.32	2
CA-CB-CG	112.60	107.79	1
CA-CB-CG	112.60	107.80	1
CB-CG-CD	112.60	104.44	1
N-CA-CB	110.50	102.34	2
C-CA-CB	110.10	100.98	1
C-N-CA	121.70	113.08	1
CB-CG-CD	112.60	104.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	109.02	2
C-CA-CB	110.10	101.03	1
C-N-CA	121.70	130.29	1
C-N-CA	121.70	113.12	1
C-N-CA	121.70	130.28	1
C-N-CA	121.70	113.13	1
CA-CB-CG	112.60	107.84	1
N-CA-CB	110.50	102.41	1
N-CA-C	112.10	100.21	2
CD2-NE2-C-N-CA	121.70	113.15	1
CA-CB-CG	112.60	107.85	1
N-CA-CB	110.50	102.43	1
CA-CB-CG	112.60	107.86	2
CA-CB-CA-CB-N-CA-CB	110.50	102.51	1
C-N-CA	121.70	130.15	1
CD2-NE2-N-CA-CB	110.50	102.53	1
CA-CB-CG	112.60	107.92	2
C-N-CA	121.70	130.12	1
N-CA-C	112.10	100.43	2
N-CA-CB	110.50	102.57	1
N-CA-C	111.00	97.96	1
N-CA-CB	110.50	102.59	1
N-CA-CB	110.50	102.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	123.86	1
N-CA-CB	110.50	102.61	1
N-CA-C	111.00	98.01	1
C-N-N-CA-CB	110.50	102.63	1
C-N-N-CA-CB	110.50	118.35	1
CD2-NE2-CE1	109.00	104.38	1
N-CA-CB	110.50	102.67	1
CA-CB-C-CA-CB	110.10	101.36	1
CD2-NE2-CE1	109.00	104.40	1
N-CA-CB	110.50	118.30	1
CA-CB-CG	112.60	108.01	1
CA-CB-CG	113.80	109.22	3
C-N-CA	121.70	113.46	1
N-CA-CB	110.50	102.72	1
CA-CB-CG	112.60	108.02	1
CA-C-N	116.90	123.76	1
C-CA-CB	110.10	101.41	1
N-CA-CB	110.50	102.74	1
CA-CB-CG	112.60	108.04	1
C-N-CA	121.70	113.50	3
CA-CB-CG	113.80	109.25	1
C-CA-CB	111.60	102.49	1
CD2-NE2-CE1	109.00	104.45	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CD2-NE2-CE1	109.00	104.45	1
CA-CB-CG	112.60	108.05	1
CA-CB-CG	112.60	108.06	2
CD2-NE2-CE1	109.00	104.46	1
CA-CB-N-CA-CB	110.50	102.78	1
CA-CB-CA-CB-CG	112.60	108.06	1
CD2-NE2-CE1	109.00	104.47	1
CA-CB-CG	112.60	108.07	4
C-CA-CB	111.60	102.54	1
N-CA-CB	110.50	102.80	1
N-CA-CB	110.50	102.81	1
N-CA-CB	110.50	118.19	1
CA-CB-CG	113.80	109.28	1
CA-CB-CD2-NE2-CE1	109.00	104.48	1
N-CA-CB	110.50	102.82	1
CD2-NE2-CD2-NE2-CE1	109.00	104.48	1
C-N-CA	121.70	129.82	1
CB-CG-CD	112.60	104.93	1
CD2-NE2-CD2-NE2-N-CA-C	111.00	123.61	1
CA-CB-CG	113.80	109.30	2
CB-CG-CD	112.60	104.95	1
N-CA-CB	110.50	102.85	1
N-CA-C	111.00	123.59	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	104.51	3
N-CA-CB	110.50	118.14	1
N-CA-CB	110.50	102.86	1
N-CA-CB	110.50	102.87	1
CA-CB-CD2-NE2-CE1	109.00	104.51	1
C-N-CA	121.70	129.77	1
CD2-NE2-CE1	109.00	104.52	4
N-CA-CA-CB-CA-C-N	116.20	125.16	1
N-CA-CB	110.50	102.89	1
C-CA-C-N-CA	121.70	129.76	1
CA-CB-CG	112.60	108.12	1
CD2-NE2-CE1	109.00	104.53	2
N-CA-CB	110.50	102.90	1
C-CA-CD2-NE2-N-CA-CB	110.50	102.90	1
CA-C-N	116.20	125.13	1
CB-CG-CD	112.60	105.01	1
CA-CB-CG	113.80	109.33	1
CD2-NE2-N-CA-C	111.00	123.50	1
CD2-NE2-CE1	109.00	104.54	1
CA-CB-CA-CB-CA-CB-CD2-NE2-CE1	109.00	104.54	1
CB-CG-CD	112.60	105.02	1
C-N-CA	121.70	129.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	110.74	97.38	1
N-CA-CD2-NE2-N-CA-C	111.00	123.45	1
CD2-NE2-CE1	109.00	104.56	3
N-CA-C	110.74	97.41	1
CA-CB-CG	112.60	108.16	3
CD2-NE2-CD2-NE2-CD2-NE2-CD2-NE2-CE1	109.00	104.56	1
CD2-NE2-CE1	109.00	104.57	1
CD2-NE2-N-CA-CB	110.50	102.99	1
CA-CB-CG	112.60	108.18	1
CD2-NE2-CD2-NE2-CA-CB-CD2-NE2-CA-CB-CA-CB-CG	112.60	108.19	1
C-CA-CB	110.10	118.48	2
CA-CB-CG	113.90	105.97	1
CD2-NE2-CE1	109.00	104.60	2
C-N-C-N-CA	121.70	129.62	1
CD2-NE2-CD2-NE2-CE1	109.00	104.60	1
CD2-NE2-CE1	109.00	104.61	4
CD2-NE2-CD2-NE2-CE1	109.00	104.61	2
CA-CB-C-N-CA-CB-CG	113.90	106.01	1
CA-CB-CD2-NE2-CD2-NE2-CD2-NE2-CE1	109.00	104.62	1
N-CA-C	111.00	123.25	1
CD2-NE2-CA-CB-CG	112.60	108.23	1
CD2-NE2-CD2-NE2-CA-CB-CG	112.60	108.24	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	123.21	1
CD2-NE2-CA-CB-CG	112.60	108.25	1
CA-CB-CG	112.60	108.25	2
CD2-NE2-CE1	109.00	104.65	1
C-N-CA	121.70	129.53	1
CA-CB-N-CA-CB	110.50	117.87	1
N-CA-CA-CB-N-CA-CB	110.50	117.86	1
CD2-NE2-CD2-NE2-CE1	109.00	104.68	1
N-CA-CD2-NE2-CD-NE-CD2-NE2-CE1	109.00	104.69	1
CA-CB-CG	113.80	109.49	1
C-CA-C-CA-CA-CB-CD2-NE2-CE1	109.00	104.70	1
CA-CB-CG	113.80	109.50	1
CA-CB-C-CA-CB	110.10	101.94	1
CA-CB-CG	112.60	108.31	1
CD-NE-C-CA-CB	110.10	102.00	1
CA-CB-CA-CB-CA-CB-CG	112.60	108.35	1
CA-CB-CG	112.60	108.35	1
CA-CB-CG	112.60	108.36	1
C-N-C-N-N-CA-CB	110.50	103.30	1
C-CA-N-CA-C	112.10	101.54	1
N-CA-C	112.10	101.54	1
C-N-CA	121.70	129.30	1
C-CA-C-N-CA	121.70	129.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-N-CA-CB	110.50	117.65	1
N-CA-CB	110.50	117.65	1
C-CA-CB	110.10	102.11	1
CA-CB-N-CA-CB	110.50	103.36	1
CA-CB-CG	112.60	108.41	1
C-CA-CB	110.10	102.16	1
CA-CB-CA-CB-CG	112.60	108.44	1
C-CA-C-CA-C-CA-CB	109.10	118.22	1
C-N-CA	121.70	129.16	1
CA-CB-CG	112.60	108.46	1
CD-NE-CZ	124.40	118.60	1
C-N-CA	121.70	129.15	1
C-N-C-N-CA	121.70	129.14	1
N-CA-C	110.74	98.34	1
C-N-CA	121.70	114.27	1
N-CA-C	110.74	98.36	1
CA-CB-CG	113.90	106.47	1
C-CA-CB	109.10	118.17	1
CA-CB-CG	112.60	108.48	1
CA-CB-CA-CB-CG	112.60	108.48	1
N-CA-CB	110.50	117.50	1
C-N-CA	121.70	114.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	107.52	2
C-N-CA	121.70	129.09	1
CD-NE-CZ	124.40	118.65	1
C-N-N-CA-CB	110.50	117.47	1
CA-CB-CG	112.60	108.50	1
CA-CB-CG	113.90	106.53	1
N-CA-C	110.74	98.49	1
CA-CB-N-CA-C	111.00	99.58	1
N-CA-CB	110.50	103.56	1
O-C-N	123.00	129.53	2
C-N-CA	121.70	114.37	2
N-CA-C	110.74	98.52	1
CA-C-N	116.90	110.79	1
C-N-C-N-N-CA-C	111.00	99.61	1
CA-CB-CA-CB-N-CA-CB	110.50	117.40	1
N-CA-CB	110.50	103.60	1
CA-CB-CG	112.60	108.55	2
CA-C-N	116.90	110.82	1
CA-CB-CG	112.60	108.56	1
CA-CB-ND1-CE1-NE2	108.40	112.43	1
ND1-CE1-NE2	108.40	112.43	1
N-CA-CB	110.50	117.34	1
N-CA-C	111.00	122.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	114.47	1
CA-CB-CG	112.60	108.58	1
CA-CB-CA-CB-CG	112.60	116.61	1
N-CA-C	111.00	122.22	1
C-N-CA	121.70	128.91	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	712.54	9139
2	635.26	8139

All 17278 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	1362	1257	84	21
2	1362	1257	84	21

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	1179	1038	94	47
2	1179	1037	95	47

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	42	0.0GLU
1	A	84	0.0ARG
1	A	131	0.0ARG
1	A	133	0.0GLN
1	A	151	0.0LEU
1	A	182	0.0LYS
1	A	211	0.0GLU
1	A	227	0.0LEU
1	A	255	0.0LYS
1	A	355	0.0GLN
1	A	360	0.0ARG
1	A	472	0.0MET
1	A	473	0.0LYS
1	A	537	0.0ARG
1	A	589	0.0LEU
1	A	596	0.0ARG
1	A	607	0.0LYS
1	A	608	0.0ILE
1	A	622	0.0LEU
1	A	628	0.0ILE
1	A	638	0.0LEU
1	A	669	0.0GLU
1	A	684	0.0VAL

Model ID	Chain	Residue ID	Residue type
1	A	707	0.0GLN
1	A	710	0.0LYS
1	A	744	0.0ARG
1	A	764	0.0GLU
1	A	769	0.0ILE
1	A	777	0.0LYS
1	A	794	0.0LYS
1	A	816	0.0ILE
1	A	867	0.0ARG
1	A	903	0.0ARG
1	A	964	0.0ARG
1	A	977	0.0HIS
1	A	978	0.0ILE
1	A	1034	0.0LYS
1	A	1040	0.0ARG
1	A	1044	0.0LEU
1	A	1073	0.0LEU
1	A	1090	0.0GLU
1	A	1094	0.0ILE
1	A	1161	0.0HIS
1	A	1198	0.0ASP
1	A	1275	0.0GLN
1	A	1286	0.0LEU



Model ID	Chain	Residue ID	Residue type
1	A	1293	0.0LEU
2	A	42	0.0GLU
2	A	84	0.0ARG
2	A	131	0.0ARG
2	A	133	0.0GLN
2	A	151	0.0LEU
2	A	182	0.0LYS
2	A	211	0.0GLU
2	A	227	0.0LEU
2	A	255	0.0LYS
2	A	355	0.0GLN
2	A	360	0.0ARG
2	A	472	0.0MET
2	A	473	0.0LYS
2	A	537	0.0ARG
2	A	589	0.0LEU
2	A	596	0.0ARG
2	A	607	0.0LYS
2	A	608	0.0ILE
2	A	622	0.0LEU
2	A	628	0.0ILE
2	A	638	0.0LEU
2	A	669	0.0GLU

Model ID	Chain	Residue ID	Residue type
2	A	684	0.0VAL
2	A	707	0.0GLN
2	A	710	0.0LYS
2	A	744	0.0ARG
2	A	764	0.0GLU
2	A	769	0.0ILE
2	A	777	0.0LYS
2	A	794	0.0LYS
2	A	816	0.0ILE
2	A	867	0.0ARG
2	A	903	0.0ARG
2	A	964	0.0ARG
2	A	977	0.0HIS
2	A	978	0.0ILE
2	A	1034	0.0LYS
2	A	1040	0.0ARG
2	A	1044	0.0LEU
2	A	1073	0.0LEU
2	A	1090	0.0GLU
2	A	1094	0.0ILE
2	A	1161	0.0HIS
2	A	1198	0.0ASP
2	A	1275	0.0GLN

Model ID	Chain	Residue ID	Residue type
2	A	1286	0.0LEU
2	A	1293	0.0LEU

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

#### 3DEM volume

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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