

# Integrative Structure Validation Report ?

March 27, 2025 - 10:01 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	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
Deposited on	2020-07-10

*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](mailto:helpdesk@pdb-ihm.org)*

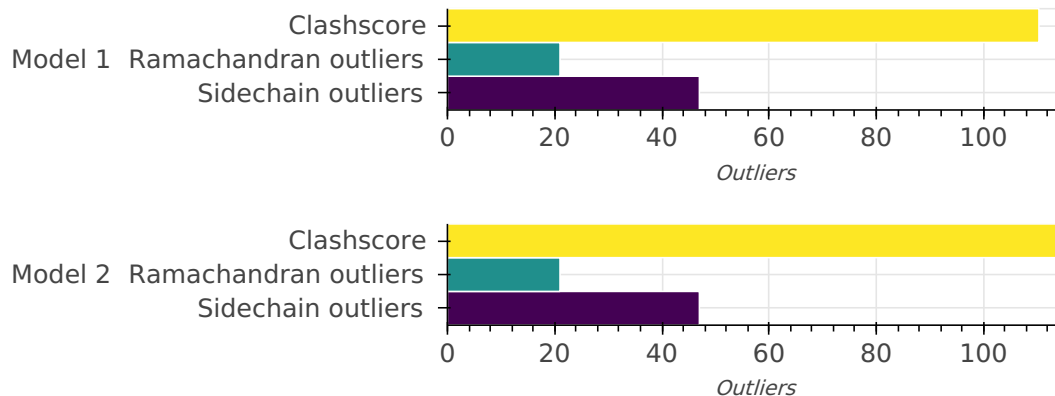
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 2 model(s). A total of 7 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	1-2	1	TdUGGT	A	1368	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	-	100.00 / 100.00	Atomic
		2	Fab Heavy Chain	B [L]	214	1-214	-	100.00 / 100.00	Atomic

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		3	Fab Light Chain	C [H]	214	1-214	-	100.00 / 100.00	Atomic

### 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	<a href="#">EMD-30386</a>
2	Other	Not available	<a href="#">10.1038/s41598-017-12283-w</a>
3	Experimental model	PDB	<a href="#">5Y7O</a>
4	Experimental model	PDB	<a href="#">5MU1</a>
5	Experimental model	PDB	<a href="#">5H18</a>
6	Experimental model	PDB	<a href="#">1FGN</a>
None	Other	Not available	Not available

### 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	Fitting the TdUGGT and Fab models in the negative stain EM map	None	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, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

### Standard geometry: bond outliers ?

*There are 22 bond length outliers in this entry (0.08% of 26410 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	629	SER	CA-C	5.34	1.41	1.52	1	2
A	950	GLU	N-CA	4.88	1.37	1.46	1	2
A	216	ARG	CA-C	4.86	1.42	1.52	2	2
A	638	LEU	N-CA	4.60	1.37	1.46	1	2
B	83	UNK	CA-CB	4.58	1.62	1.53	1	2
A	628	ILE	CA-C	4.49	1.43	1.52	1	2
A	612	ASN	CA-C	4.43	1.43	1.52	1	2
A	216	ARG	N-CA	4.40	1.37	1.46	2	2
A	1133	LEU	C-N	4.28	1.39	1.33	1	2
A	928	LEU	C-N	4.20	1.27	1.34	1	2
A	84	ARG	NE-CZ	4.11	1.37	1.33	1	2

### Standard geometry: angle outliers ?

*There are 628 bond angle outliers in this entry (1.74% of 36006 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	637	SER	C-N-CA	21.71	82.62	121.70	2	2
A	1180	PHE	CA-CB-CG	11.38	102.42	113.80	1	2
A	912	PHE	CA-CB-CG	11.13	102.67	113.80	1	2
A	979	LEU	C-N-CA	10.92	102.04	121.70	2	2
A	1233	PHE	CA-CB-CG	10.92	102.88	113.80	1	2
A	1068	PHE	CA-CB-CG	10.81	102.99	113.80	1	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	612	ASN	CA-CB-CG	10.02	102.58	112.60	2	2
A	646	PHE	CA-CB-CG	9.95	103.85	113.80	1	2
A	216	ARG	C-N-CA	9.82	104.03	121.70	1	2
A	1132	PHE	CA-CB-CG	9.62	104.18	113.80	2	2
A	204	PHE	CA-CB-CG	8.86	104.94	113.80	2	2
A	812	THR	C-N-CA	8.75	137.45	121.70	2	2
A	950	GLU	N-CA-CB	8.73	95.65	110.50	1	2
A	1134	SER	CA-C-N	8.67	129.90	116.90	1	2
A	223	ASP	C-N-CA	8.08	107.15	121.70	1	2
C	56	UNK	N-CA-C	8.03	134.83	110.74	1	2
A	821	PHE	CA-CB-CG	7.76	106.04	113.80	2	2
A	1133	LEU	C-N-CA	7.71	135.57	121.70	1	2
A	595	THR	C-N-CA	7.62	107.98	121.70	2	2
A	12	PHE	CA-CB-CG	7.59	106.21	113.80	1	2
A	699	ALA	C-CA-CB	7.55	99.18	110.50	1	2
A	432	PHE	CA-CB-CG	7.36	106.44	113.80	1	2
A	396	TYR	CA-CB-CG	7.33	100.70	113.90	1	2
A	170	PHE	CA-CB-CG	7.29	106.51	113.80	1	2
A	596	ARG	C-N-CA	7.00	134.31	121.70	2	2
A	260	PHE	CA-CB-CG	6.99	106.81	113.80	2	2
A	813	THR	C-N-CA	6.98	134.26	121.70	2	2
A	466	HIS	CA-CB-CG	6.98	106.82	113.80	2	2
A	1074	PHE	CA-CB-CG	6.95	106.85	113.80	1	2
A	223	ASP	CA-CB-CG	6.94	105.66	112.60	2	2
A	832	ILE	C-N-CA	6.89	109.30	121.70	2	2
A	1148	TYR	CA-CB-CG	6.83	101.61	113.90	1	2
A	1137	PHE	CA-CB-CG	6.80	107.00	113.80	1	2
A	259	ASP	CA-CB-CG	6.80	105.80	112.60	2	2
A	1185	PHE	CA-CB-CG	6.74	107.06	113.80	1	2
A	1008	PHE	CA-CB-CG	6.64	107.16	113.80	2	2
A	250	PHE	CA-CB-CG	6.63	107.17	113.80	1	2
A	381	TYR	CA-CB-CG	6.55	102.10	113.90	2	2
A	1194	PHE	CA-CB-CG	6.55	107.25	113.80	1	2
A	384	PHE	CA-CB-CG	6.54	107.26	113.80	1	2
A	950	GLU	C-CA-CB	6.45	122.36	110.10	1	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	200	PHE	CA-CB-CG	6.43	107.37	113.80	2	2
C	131	UNK	N-CA-C	6.35	91.69	110.74	1	2
A	82	ALA	C-N-CA	6.32	133.08	121.70	2	2
A	898	ILE	C-N-CA	6.27	132.98	121.70	2	2
A	689	TYR	CA-CB-CG	6.26	102.64	113.90	2	2
A	1126	PHE	CA-CB-CG	6.25	107.55	113.80	2	2
A	901	PHE	CA-CB-CG	6.23	107.57	113.80	1	2
A	326	PHE	CA-CB-CG	6.19	107.61	113.80	1	2
A	519	GLU	CB-CG-CD	6.13	102.18	112.60	1	2
A	276	PHE	CA-CB-CG	6.11	107.69	113.80	2	2
A	1140	PHE	CA-CB-CG	6.11	107.69	113.80	1	2
C	136	UNK	N-CA-C	6.10	92.44	110.74	1	2
A	628	ILE	N-CA-C	6.08	93.98	111.00	2	2
A	475	PHE	CA-CB-CG	6.05	107.75	113.80	1	2
A	699	ALA	N-CA-CB	6.01	119.42	110.40	1	2
A	1053	GLN	CA-C-N	6.00	125.90	116.90	2	2
A	1052	TYR	CA-CB-CG	5.99	103.12	113.90	2	2
A	94	TYR	C-N-CA	5.98	110.94	121.70	2	2
A	441	PHE	CA-CB-CG	5.95	107.85	113.80	1	2
A	647	ASP	CA-CB-CG	5.92	106.68	112.60	1	2
B	140	UNK	C-N-CA	5.89	132.30	121.70	2	2
A	533	ASP	CA-CB-CG	5.86	106.74	112.60	1	2
A	245	ASP	CA-CB-CG	5.85	106.75	112.60	1	2
A	420	ASP	CA-CB-CG	5.84	106.76	112.60	2	2
A	1119	HIS	CA-CB-CG	5.82	107.98	113.80	1	2
A	636	ASN	CA-CB-CG	5.81	106.79	112.60	2	2
A	738	GLY	N-CA-C	5.81	96.45	113.30	2	2
A	565	ASP	CA-CB-CG	5.80	106.80	112.60	2	2
C	153	UNK	N-CA-CB	5.80	100.64	110.50	2	2
A	604	ASP	CA-C-N	5.79	125.59	116.90	1	2
A	73	ASP	N-CA-CB	5.76	120.30	110.50	2	2
A	305	ARG	C-N-CA	5.73	132.02	121.70	1	2
A	801	PHE	CA-CB-CG	5.70	108.10	113.80	1	2
A	217	THR	O-C-N	5.68	113.92	123.00	1	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	217	THR	C-CA-CB	5.66	121.55	109.10	1	2
A	595	THR	N-CA-C	5.65	126.83	111.00	2	2
A	1270	ASP	CA-CB-CG	5.64	106.96	112.60	1	2
A	1065	LEU	C-N-CA	5.62	131.81	121.70	1	2
A	120	ASP	CA-CB-CG	5.62	106.98	112.60	1	2
A	446	LEU	C-N-CA	5.60	131.78	121.70	1	2
A	653	ASN	CA-CB-CG	5.60	107.00	112.60	1	2
A	88	PRO	C-CA-CB	5.60	120.74	110.10	1	2
A	1155	VAL	C-N-CA	5.59	131.76	121.70	1	2
A	629	SER	N-CA-C	5.53	95.52	111.00	2	2
A	258	GLN	C-N-CA	5.52	131.64	121.70	1	2
A	836	ASN	CA-CB-CG	5.48	107.12	112.60	1	2
A	64	ASP	CA-CB-CG	5.48	107.12	112.60	1	2
A	614	VAL	C-CA-CB	5.46	101.02	111.40	1	2
A	661	PHE	CA-CB-CG	5.45	108.35	113.80	1	2
A	361	ASP	CA-CB-CG	5.44	107.16	112.60	1	2
A	1093	ASP	CA-CB-CG	5.43	107.17	112.60	2	2
A	218	ASP	N-CA-CB	5.42	119.72	110.50	1	2
A	1020	PHE	CA-CB-CG	5.41	108.39	113.80	1	2
A	498	SER	C-N-CA	5.41	131.44	121.70	2	2
A	343	PRO	C-N-CA	5.39	112.00	121.70	2	2
A	886	PHE	CA-CB-CG	5.38	108.42	113.80	2	2
A	95	GLN	N-CA-CB	5.36	119.60	110.50	2	2
A	957	ASN	CA-CB-CG	5.35	107.25	112.60	1	2
A	283	ASN	CA-CB-CG	5.34	107.26	112.60	2	2

### 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	110.34	2664
2	114.27	2759

There are 5423 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:430:GLN:CB	C:101:UNK:CB	1.57	2	1
A:435:ARG:HD3	C:31:UNK:CB	1.50	2	1
A:395:THR:HG23	C:27:UNK:CA	1.50	1	1
A:500:ARG:CB	B:29:UNK:HA	1.47	2	1
A:481:LYS:HE2	B:64:UNK:N	1.43	2	1
A:401:PRO:HD3	C:30:UNK:CB	1.40	1	1
A:435:ARG:CD	C:31:UNK:CB	1.40	2	1
A:430:GLN:HB3	C:101:UNK:CB	1.37	2	1
A:500:ARG:HB3	B:29:UNK:CA	1.35	2	1
A:481:LYS:CE	B:64:UNK:N	1.35	2	1
A:401:PRO:CA	C:30:UNK:O	1.35	1	1
A:385:PRO:HD2	C:57:UNK:CB	1.34	1	1
A:395:THR:CB	C:27:UNK:CB	1.34	1	1
A:430:GLN:NE2	C:101:UNK:C	1.34	2	1
A:476:GLN:O	B:53:UNK:CB	1.33	2	1
A:436:LEU:C	C:30:UNK:O	1.29	2	1
A:430:GLN:HE21	C:101:UNK:C	1.28	2	1
A:434:LYS:O	C:32:UNK:C	1.26	2	1
A:403:VAL:HG22	C:55:UNK:CB	1.26	1	1
A:385:PRO:CD	C:57:UNK:CB	1.25	1	1
A:498:SER:C	B:30:UNK:CB	1.25	2	1
A:477:ARG:HD2	B:51:UNK:CB	1.24	2	1
A:435:ARG:O	C:30:UNK:C	1.23	2	1
A:384:PHE:CD1	C:55:UNK:CB	1.23	2	1
A:481:LYS:HE2	B:64:UNK:CA	1.23	2	1
A:368:VAL:HG13	A:525:THR:HG22	1.20	2	2
A:434:LYS:O	C:33:UNK:N	1.19	2	1
A:501:VAL:HA	B:92:UNK:O	1.16	2	1
A:430:GLN:NE2	C:102:UNK:N	1.16	2	1
A:476:GLN:HB2	B:50:UNK:CB	1.16	2	1
A:401:PRO:N	C:30:UNK:O	1.15	1	1
A:630:ALA:HB2	A:699:ALA:HB2	1.15	1	2
A:436:LEU:HB3	C:54:UNK:CB	1.15	2	1
A:401:PRO:HG3	C:30:UNK:CA	1.15	1	1
A:401:PRO:CD	C:30:UNK:CB	1.15	1	1



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:477:ARG:CD	B:51:UNK:CB	1.14	2	1
A:340:LEU:HD13	A:343:PRO:HG2	1.13	2	2
A:521:VAL:HA	A:524:LYS:HE3	1.13	2	2
A:435:ARG:CG	C:31:UNK:CB	1.13	2	1
A:393:GLN:HG2	C:77:UNK:N	1.12	1	1
A:431:THR:HA	C:100:UNK:HA	1.12	2	1
A:158:LEU:HD21	A:160:ILE:HD11	1.12	2	2
A:384:PHE:HD1	C:55:UNK:CB	1.12	2	1
A:877:LYS:HD2	A:908:PRO:HG2	1.11	2	2
A:473:LYS:HD3	B:31:UNK:C	1.11	2	1
A:437:ILE:N	C:31:UNK:HA	1.11	2	1
A:498:SER:O	B:30:UNK:CB	1.11	2	1
A:794:LYS:HA	A:794:LYS:HE3	1.11	1	2
A:217:THR:HG23	A:225:LYS:HA	1.11	2	2
A:401:PRO:HG3	C:30:UNK:HA	1.10	1	1
A:388:ILE:HG12	A:573:ILE:HD12	1.10	1	2
A:1117:MET:HA	A:1117:MET:HE2	1.10	1	2
A:638:LEU:HB3	A:668:ILE:HG12	1.10	1	2
A:690:GLN:HG2	A:693:ARG:HD2	1.09	1	2
A:462:LEU:HD22	A:471:MET:HA	1.09	2	2
A:401:PRO:HA	C:30:UNK:O	1.09	1	1
A:350:SER:HB3	A:827:TYR:HA	1.09	1	2
A:353:GLU:HB3	A:355:GLN:HE22	1.09	2	2
A:99:THR:HG22	A:1002:THR:HG23	1.08	2	2
A:382:SER:CB	C:55:UNK:O	1.08	2	1
A:1134:SER:HB3	A:1137:PHE:HB2	1.08	1	2
A:69:ASN:HA	A:74:LEU:HD21	1.08	2	2
A:950:GLU:HG3	A:1133:LEU:HB2	1.08	2	2
A:732:GLN:HG3	A:733:LEU:HD22	1.08	2	2
A:436:LEU:O	C:30:UNK:O	1.08	2	1
A:869:VAL:HG23	A:870:PRO:HD3	1.08	1	2
A:1163:LEU:HD21	A:1179:LEU:HD23	1.07	2	2
A:72:ALA:HB1	A:320:ARG:HH21	1.07	2	2
A:529:ILE:HG23	A:534:LEU:HB2	1.07	2	2
A:622:LEU:HD21	A:626:LEU:HD11	1.07	1	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:434:LYS:HD2	C:32:UNK:CA	1.07	2	1
A:345:LEU:HD23	A:778:ARG:HA	1.07	2	2
A:1047:VAL:HG11	A:1073:LEU:HD23	1.07	2	2
A:622:LEU:HD13	A:733:LEU:HB2	1.06	1	2
A:434:LYS:HD2	C:32:UNK:CB	1.05	2	1
A:391:LEU:HD21	A:400:LEU:HD22	1.05	2	2
A:460:ARG:HG3	A:464:MET:HE3	1.05	2	2
A:279:GLU:HA	A:282:ALA:HB3	1.05	2	2
A:607:LYS:HE3	A:609:ARG:HG3	1.05	2	2
A:434:LYS:NZ	C:32:UNK:CB	1.05	2	1
A:613:LEU:HD13	A:802:ALA:HB1	1.04	2	2
A:893:LEU:HD13	A:897:PRO:HG3	1.04	1	2
A:858:ILE:HD13	A:885:ILE:HG23	1.04	2	2
A:600:ILE:HG23	A:770:LEU:HD13	1.03	2	2
A:748:LEU:HD12	A:774:GLU:HG2	1.03	1	2
A:662:ARG:HE	A:669:GLU:HG3	1.03	2	2
A:227:LEU:HD13	A:228:SER:H	1.03	2	2
A:20:GLU:HB2	A:86:ALA:HB3	1.03	2	2
A:1114:VAL:HG21	A:1358:ILE:HD11	1.03	1	2
A:743:THR:HG23	A:755:PRO:HB3	1.02	2	2
A:501:VAL:HG13	B:92:UNK:CA	1.02	2	1
A:997:GLN:HB2	A:1034:LYS:HD2	1.02	2	2
A:382:SER:HB2	C:55:UNK:O	1.02	2	1
A:979:LEU:HD13	A:1065:LEU:HA	1.02	1	2
A:650:ALA:HA	A:653:ASN:HB2	1.02	2	2
A:647:ASP:HB2	A:721:SER:HA	1.01	2	2
A:814:SER:HA	A:826:LYS:HD2	1.01	2	2
A:494:GLU:HB3	B:67:UNK:CB	1.01	2	1
A:682:THR:HG23	A:722:LYS:HA	1.01	1	2
A:476:GLN:OE1	B:50:UNK:CB	1.01	2	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	1362	1257	84	21

Model ID	Analysed	Favored	Allowed	Outliers
2	1362	1257	84	21

There are 21 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	47	ASP	2
A	107	THR	2
A	136	VAL	2
A	216	ARG	2
A	227	LEU	2
A	340	LEU	2
A	355	GLN	2
A	382	SER	2
A	400	LEU	2
A	594	LEU	2
A	725	ALA	2
A	776	SER	2
A	786	MET	2
A	791	LEU	2
A	793	HIS	2
A	848	ASP	2
A	898	ILE	2
A	1053	GLN	2
A	1059	GLU	2
A	1214	GLU	2
A	1331	CYS	2

### 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	1179	1038	94	47
2	1179	1037	95	47

There are 47 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	42	GLU	2

Chain	Res	Type	Models (Total)
A	84	ARG	2
A	131	ARG	2
A	133	GLN	2
A	151	LEU	2
A	182	LYS	2
A	211	GLU	2
A	227	LEU	2
A	255	LYS	2
A	355	GLN	2
A	360	ARG	2
A	472	MET	2
A	473	LYS	2
A	537	ARG	2
A	589	LEU	2
A	596	ARG	2
A	607	LYS	2
A	608	ILE	2
A	622	LEU	2
A	628	ILE	2
A	638	LEU	2
A	669	GLU	2
A	684	VAL	2
A	707	GLN	2
A	710	LYS	2
A	744	ARG	2
A	764	GLU	2
A	769	ILE	2
A	777	LYS	2
A	794	LYS	2
A	816	ILE	2
A	867	ARG	2
A	903	ARG	2
A	964	ARG	2
A	977	HIS	2
A	978	ILE	2

Chain	Res	Type	Models (Total)
A	1034	LYS	2
A	1040	ARG	2
A	1044	LEU	2
A	1073	LEU	2
A	1090	GLU	2
A	1094	ILE	2
A	1161	HIS	2
A	1198	ASP	2
A	1275	GLN	2
A	1286	LEU	2
A	1293	LEU	2

### 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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