

Integrative Structure Validation Report ?

February 18, 2025 - 08:37 AM PST

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	9A3G
PDB-Dev ID	PDBDEV_00000201
Structure Title	Invariant surface glycoprotein 65 of Trypanosoma brucei gambiense
Structure Authors	Suelzen, H.; Zoll, S.
Deposited on	2023-02-16

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

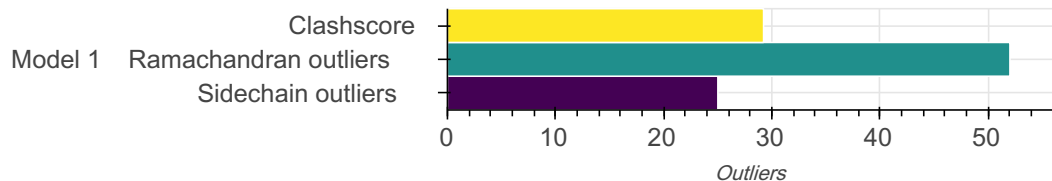
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 5 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	Invariant surface glycoprotein 65	A	420	-	1-18, 19-129, 130-186, 187-210, 211-239, 240-296, 297-420	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	3DEM volume	EMDB	EMD-14707
5	Mass Spectrometry data	PRIDE	PXD033606
1	Experimental model	PDB	7ZGJ
3	De Novo model	Not available	Not available
4	De Novo model	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	AlphaFold model prediction	None	None	None	False	False
2	1	Modelling	None	None	None	False	False
3	1	Refinement	None	None	None	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaFold2	Not available	protein structure prediction	https://www.deepmind.com/research/highlighted-research/alphafold
2	Coot	Not available	model building	https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/
3	Phenix	Not available	refinement	https://phenix-online.org/

Data quality ?

Mass Spectrometry

Validation for this section is under development.

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 45 bond length outliers in this entry (1.36% of 3318 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	18	LEU	C-N	45.94	1.97	1.33	1	1
A	302	LYS	C-N	35.14	0.84	1.33	1	1
A	186	SER	C-N	31.70	1.77	1.33	1	1
A	296	ALA	C-N	22.10	1.64	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	327	PRO	N-CD	11.23	1.63	1.47	1	1
A	309	PRO	N-CD	10.95	1.32	1.47	1	1
A	404	VAL	C-N	9.95	1.47	1.33	1	1
A	326	ALA	C-N	9.92	1.50	1.34	1	1
A	313	PRO	N-CD	9.67	1.34	1.47	1	1
A	368	ARG	C-N	7.66	1.22	1.33	1	1
A	303	GLY	C-N	7.53	1.43	1.33	1	1
A	353	LEU	C-N	7.06	1.23	1.33	1	1
A	386	THR	C-N	6.81	1.23	1.33	1	1
A	305	LYS	C-N	6.67	1.42	1.33	1	1
A	383	LEU	C-N	6.38	1.24	1.33	1	1
A	336	ALA	C-N	6.31	1.42	1.33	1	1
A	379	PRO	C-N	6.19	1.24	1.33	1	1
A	332	ASP	C-N	5.87	1.41	1.33	1	1
A	379	PRO	N-CD	5.64	1.39	1.47	1	1
A	321	LYS	C-N	5.56	1.41	1.33	1	1
A	331	VAL	C-N	5.55	1.41	1.33	1	1
A	381	ILE	C-N	5.45	1.25	1.33	1	1
A	327	PRO	C-N	5.44	1.41	1.33	1	1
A	418	VAL	C-N	5.33	1.25	1.33	1	1
A	362	VAL	C-N	5.02	1.26	1.33	1	1
A	351	ASP	C-N	4.90	1.26	1.33	1	1
A	369	THR	C-N	4.87	1.26	1.33	1	1
A	357	THR	C-N	4.86	1.26	1.33	1	1
A	373	ILE	C-N	4.85	1.26	1.33	1	1
A	335	ILE	C-N	4.72	1.40	1.33	1	1
A	339	GLU	C-N	4.69	1.26	1.33	1	1
A	400	ASN	C-N	4.68	1.39	1.33	1	1
A	376	VAL	C-N	4.65	1.26	1.33	1	1
A	346	ILE	C-N	4.61	1.39	1.33	1	1
A	382	ILE	C-N	4.60	1.26	1.33	1	1
A	371	MET	C-N	4.60	1.26	1.33	1	1
A	344	VAL	C-N	4.38	1.39	1.33	1	1
A	315	THR	C-N	4.34	1.41	1.34	1	1
A	372	ILE	C-N	4.23	1.27	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	401	SER	C-N	4.13	1.39	1.33	1	1
A	374	LEU	C-N	4.13	1.27	1.33	1	1
A	304	ALA	C-N	4.10	1.39	1.33	1	1
A	349	ASP	C-N	4.09	1.39	1.33	1	1
A	322	ASN	C-N	4.04	1.39	1.33	1	1
A	360	ALA	C-N	4.04	1.27	1.33	1	1

Standard geometry: angle outliers ?

There are 93 bond angle outliers in this entry (2.08% of 4479 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	186	SER	O-C-N	42.51	54.99	123.00	1	1
A	18	LEU	O-C-N	33.50	69.40	123.00	1	1
A	18	LEU	C-N-CA	16.96	91.17	121.70	1	1
A	322	ASN	C-N-CA	16.09	150.66	121.70	1	1
A	413	VAL	C-N-CA	15.24	149.13	121.70	1	1
A	320	THR	C-N-CA	14.65	148.07	121.70	1	1
A	304	ALA	O-C-N	14.19	100.29	123.00	1	1
A	344	VAL	O-C-N	14.00	100.60	123.00	1	1
A	318	ASN	C-N-CA	12.67	144.50	121.70	1	1
A	335	ILE	C-N-CA	12.06	143.41	121.70	1	1
A	302	LYS	C-N-CA	12.05	100.01	121.70	1	1
A	309	PRO	O-C-N	11.83	104.07	123.00	1	1
A	402	HIS	O-C-N	11.32	104.88	123.00	1	1
A	340	THR	C-N-CA	11.22	141.89	121.70	1	1
A	339	GLU	O-C-N	11.10	105.24	123.00	1	1
A	330	HIS	C-N-CA	11.09	141.65	121.70	1	1
A	415	SER	C-N-CA	11.04	141.57	121.70	1	1
A	419	VAL	C-N-CA	10.91	141.34	121.70	1	1
A	307	ILE	O-C-N	10.88	105.59	123.00	1	1
A	345	GLY	O-C-N	10.65	105.96	123.00	1	1
A	303	GLY	O-C-N	10.59	106.05	123.00	1	1
A	343	GLU	O-C-N	10.53	106.14	123.00	1	1
A	332	ASP	C-N-CA	10.47	140.54	121.70	1	1
A	305	LYS	O-C-N	10.30	106.53	123.00	1	1
A	340	THR	O-C-N	10.09	106.86	123.00	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	417	LYS	C-N-CA	9.56	138.91	121.70	1	1
A	341	GLN	O-C-N	9.25	108.21	123.00	1	1
A	337	THR	C-N-CA	9.20	138.25	121.70	1	1
A	412	GLY	C-N-CA	9.07	138.03	121.70	1	1
A	327	PRO	CA-N-CD	8.80	99.68	112.00	1	1
A	310	ALA	O-C-N	8.66	109.15	123.00	1	1
A	403	ASP	O-C-N	8.65	109.16	123.00	1	1
A	328	THR	C-N-CA	8.58	137.15	121.70	1	1
A	323	ASP	C-N-CA	8.52	137.03	121.70	1	1
A	314	ALA	O-C-N	8.51	109.39	123.00	1	1
A	303	GLY	C-N-CA	8.29	136.62	121.70	1	1
A	306	ILE	O-C-N	8.22	109.85	123.00	1	1
A	313	PRO	O-C-N	8.11	110.03	123.00	1	1
A	405	ASP	C-N-CA	7.96	136.03	121.70	1	1
A	317	THR	O-C-N	7.95	110.27	123.00	1	1
A	342	VAL	C-N-CA	7.90	135.92	121.70	1	1
A	311	ALA	O-C-N	7.81	110.50	123.00	1	1
A	210	VAL	C-N-CA	7.43	135.07	121.70	1	1
A	186	SER	CA-C-N	7.12	130.44	116.20	1	1
A	408	LYS	C-N-CA	7.08	134.44	121.70	1	1
A	325	SER	O-C-N	7.03	111.75	123.00	1	1
A	338	ASN	C-N-CA	7.03	134.35	121.70	1	1
A	348	ALA	O-C-N	6.85	112.03	123.00	1	1
A	327	PRO	O-C-N	6.78	112.15	123.00	1	1
A	316	PRO	O-C-N	6.68	112.31	123.00	1	1
A	308	ILE	O-C-N	6.51	112.58	123.00	1	1
A	401	SER	O-C-N	6.40	112.76	123.00	1	1
A	312	ALA	O-C-N	6.39	112.78	123.00	1	1
A	343	GLU	C-N-CA	6.37	110.23	121.70	1	1
A	326	ALA	C-N-CA	6.30	154.12	122.60	1	1
A	342	VAL	O-C-N	6.20	113.07	123.00	1	1
A	184	CYS	C-CA-CB	6.17	121.82	110.10	1	1
A	328	THR	O-C-N	6.02	113.36	123.00	1	1
A	336	ALA	C-N-CA	5.77	111.31	121.70	1	1
A	407	GLY	C-N-CA	5.39	131.40	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	318	ASN	O-C-N	5.38	114.40	123.00	1	1
A	315	THR	C-N-CD	5.34	103.12	125.00	1	1
A	311	ALA	C-N-CA	5.27	131.19	121.70	1	1
A	347	ASP	O-C-N	5.17	114.73	123.00	1	1
A	314	ALA	C-N-CA	5.16	112.41	121.70	1	1
A	316	PRO	C-N-CA	5.08	130.84	121.70	1	1
A	414	SER	C-N-CA	5.00	130.70	121.70	1	1
A	18	LEU	CA-C-N	4.98	106.24	116.20	1	1
A	326	ALA	C-N-CD	4.96	104.67	125.00	1	1
A	333	ARG	C-N-CA	4.96	130.62	121.70	1	1
A	400	ASN	O-C-N	4.95	115.07	123.00	1	1
A	211	LYS	C-CA-CB	4.93	100.73	110.10	1	1
A	345	GLY	C-N-CA	4.87	112.93	121.70	1	1
A	173	HIS	CB-CG-CD2	4.83	124.93	131.20	1	1
A	346	ILE	O-C-N	4.70	115.48	123.00	1	1
A	331	VAL	O-C-N	4.67	115.52	123.00	1	1
A	404	VAL	O-C-N	4.66	115.54	123.00	1	1
A	316	PRO	CA-N-CD	4.60	105.56	112.00	1	1
A	411	GLY	O-C-N	4.57	115.69	123.00	1	1
A	338	ASN	O-C-N	4.56	115.71	123.00	1	1
A	320	THR	O-C-N	4.51	115.78	123.00	1	1
A	228	GLN	OE1-CD-NE2	4.45	118.15	122.60	1	1
A	308	ILE	CA-C-N	4.42	123.53	116.90	1	1
A	407	GLY	O-C-N	4.32	116.09	123.00	1	1
A	324	ASP	O-C-N	4.25	116.19	123.00	1	1
A	410	GLU	O-C-N	4.16	116.35	123.00	1	1
A	211	LYS	N-CA-CB	4.12	117.51	110.50	1	1
A	305	LYS	C-N-CA	4.12	129.11	121.70	1	1
A	6	GLY	O-C-N	4.12	116.41	123.00	1	1
A	397	ARG	O-C-N	4.11	116.42	123.00	1	1
A	11	ARG	NE-CZ-NH2	4.11	122.89	119.20	1	1
A	313	PRO	C-N-CA	4.08	129.04	121.70	1	1
A	304	ALA	CA-C-N	4.01	124.23	116.20	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	29.23	190

There are 190 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)
A:144:LEU:CG	A:245:TYR:OH	1.41	1	1
A:96:LYS:NZ	A:348:ALA:CB	1.38	1	1
A:144:LEU:CD1	A:245:TYR:OH	1.34	1	1
A:20:LYS:HG3	A:166:ASP:O	1.26	1	1
A:302:LYS:CA	A:303:GLY:N	1.25	1	1
A:18:LEU:C	A:19:THR:N	1.22	1	1
A:293:ILE:HD11	A:354:LEU:CD2	1.22	1	1
A:293:ILE:CD1	A:354:LEU:CD2	1.21	1	1
A:96:LYS:NZ	A:348:ALA:HB1	1.19	1	1
A:146:ARG:HB2	A:241:TRP:CZ2	1.19	1	1
A:23:ALA:HB2	A:168:ILE:CD1	1.18	1	1
A:293:ILE:CD1	A:354:LEU:HD23	1.17	1	1
A:418:VAL:O	A:419:VAL:HG23	1.17	1	1
A:186:SER:O	A:187:THR:HG23	1.16	1	1
A:96:LYS:NZ	A:348:ALA:HB2	1.16	1	1
A:336:ALA:O	A:337:THR:HG23	1.14	1	1
A:144:LEU:HG	A:245:TYR:OH	1.14	1	1
A:315:THR:HG22	A:316:PRO:HD3	1.14	1	1
A:20:LYS:HA	A:168:ILE:HG13	1.13	1	1
A:19:THR:HA	A:166:ASP:HB3	1.13	1	1
A:315:THR:HG22	A:316:PRO:CD	1.11	1	1
A:334:GLY:O	A:335:ILE:HG13	1.11	1	1
A:23:ALA:CB	A:168:ILE:HD13	1.10	1	1
A:20:LYS:CG	A:166:ASP:O	1.10	1	1
A:315:THR:CG2	A:316:PRO:HD3	1.10	1	1
A:20:LYS:N	A:166:ASP:O	1.08	1	1
A:293:ILE:HG13	A:354:LEU:HD22	1.08	1	1
A:297:LYS:HE3	A:354:LEU:HB3	1.07	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:146:ARG:HB2	A:241:TRP:CH2	1.06	1	1
A:18:LEU:HD12	A:22:GLY:HA3	1.05	1	1
A:144:LEU:HD12	A:245:TYR:OH	1.05	1	1
A:144:LEU:HD11	A:245:TYR:CE2	1.05	1	1
A:18:LEU:CD1	A:22:GLY:HA3	1.03	1	1
A:96:LYS:HZ2	A:348:ALA:HB1	1.02	1	1
A:30:LYS:HE2	A:144:LEU:O	1.02	1	1
A:293:ILE:CG1	A:354:LEU:HD22	1.02	1	1
A:293:ILE:HD11	A:354:LEU:HD23	1.02	1	1
A:23:ALA:CB	A:168:ILE:CD1	1.01	1	1
A:27:CYS:SG	A:182:ILE:HG22	1.00	1	1
A:293:ILE:CD1	A:354:LEU:HD22	1.00	1	1
A:18:LEU:O	A:19:THR:N	1.00	1	1
A:20:LYS:HA	A:168:ILE:CG1	1.00	1	1
A:144:LEU:CD1	A:245:TYR:CZ	1.00	1	1
A:20:LYS:HG3	A:166:ASP:C	0.99	1	1
A:144:LEU:HG	A:245:TYR:CZ	0.99	1	1
A:23:ALA:HB2	A:168:ILE:HD13	0.97	1	1
A:146:ARG:CB	A:241:TRP:CH2	0.95	1	1
A:96:LYS:HZ3	A:348:ALA:CB	0.93	1	1
A:186:SER:O	A:187:THR:CG2	0.93	1	1
A:30:LYS:CE	A:144:LEU:O	0.92	1	1
A:96:LYS:HZ1	A:348:ALA:HB2	0.92	1	1
A:297:LYS:CE	A:354:LEU:HB3	0.91	1	1
A:297:LYS:HG3	A:354:LEU:HD13	0.91	1	1
A:297:LYS:CG	A:354:LEU:HD13	0.91	1	1
A:96:LYS:HZ1	A:348:ALA:CB	0.88	1	1
A:336:ALA:C	A:337:THR:HG23	0.87	1	1
A:302:LYS:C	A:303:GLY:N	0.86	1	1
A:92:GLU:OE2	A:350:PHE:CZ	0.84	1	1
A:18:LEU:HD11	A:22:GLY:C	0.84	1	1
A:23:ALA:HB3	A:168:ILE:HG12	0.84	1	1
A:30:LYS:HG2	A:144:LEU:HB3	0.83	1	1
A:334:GLY:C	A:335:ILE:HG13	0.83	1	1
A:327:PRO:O	A:328:THR:HG23	0.82	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:26:LEU:HG	A:148:LEU:HD21	0.81	1	1
A:144:LEU:CD1	A:245:TYR:CE2	0.81	1	1
A:27:CYS:SG	A:182:ILE:CG2	0.81	1	1
A:129:ALA:HA	A:131:GLY:N	0.80	1	1
A:144:LEU:HD11	A:245:TYR:CZ	0.80	1	1
A:418:VAL:C	A:419:VAL:HG23	0.80	1	1
A:26:LEU:HG	A:148:LEU:CD2	0.79	1	1
A:18:LEU:CD1	A:22:GLY:CA	0.79	1	1
A:20:LYS:CA	A:168:ILE:HG13	0.77	1	1
A:96:LYS:HZ3	A:348:ALA:HB2	0.77	1	1
A:289:LEU:HB2	A:361:GLU:OE1	0.76	1	1
A:409:ALA:HB1	A:410:GLU:HG3	0.76	1	1
A:144:LEU:CG	A:245:TYR:CZ	0.75	1	1
A:203:ALA:O	A:206:SER:OG	0.75	1	1
A:145:TYR:N	A:241:TRP:CZ3	0.74	1	1
A:336:ALA:O	A:337:THR:CG2	0.72	1	1
A:418:VAL:O	A:419:VAL:CG2	0.71	1	1
A:146:ARG:CB	A:241:TRP:CZ2	0.71	1	1
A:293:ILE:HD12	A:354:LEU:CD2	0.71	1	1
A:23:ALA:HB3	A:168:ILE:CG1	0.71	1	1
A:20:LYS:CA	A:166:ASP:O	0.69	1	1
A:17:LYS:C	A:19:THR:N	0.69	1	1
A:297:LYS:CE	A:354:LEU:CB	0.68	1	1
A:194:ASP:OD1	A:196:SER:OG	0.68	1	1
A:315:THR:HG22	A:316:PRO:HD2	0.67	1	1
A:30:LYS:HE2	A:144:LEU:C	0.67	1	1
A:186:SER:C	A:187:THR:HG23	0.66	1	1
A:373:ILE:CG2	A:377:LEU:HD12	0.66	1	1
A:19:THR:OG1	A:21:GLU:OE1	0.66	1	1
A:86:ASP:OD1	A:289:LEU:HB3	0.64	1	1
A:402:HIS:O	A:403:ASP:HB2	0.64	1	1
A:85:SER:OG	A:89:LYS:NZ	0.64	1	1
A:144:LEU:HD11	A:245:TYR:HE2	0.64	1	1
A:18:LEU:CD1	A:22:GLY:C	0.64	1	1
A:297:LYS:HG2	A:354:LEU:HD13	0.64	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:18:LEU:HD11	A:22:GLY:CA	0.63	1	1
A:23:ALA:HB3	A:168:ILE:CD1	0.63	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	418	322	44	52

There are 52 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	2	LEU	1
A	3	LEU	1
A	7	SER	1
A	8	GLU	1
A	18	LEU	1
A	19	THR	1
A	129	ALA	1
A	176	SER	1
A	187	THR	1
A	211	LYS	1
A	290	THR	1
A	304	ALA	1
A	305	LYS	1
A	309	PRO	1
A	310	ALA	1
A	311	ALA	1
A	312	ALA	1
A	314	ALA	1
A	317	THR	1
A	319	SER	1
A	321	LYS	1
A	322	ASN	1
A	323	ASP	1
A	324	ASP	1
A	325	SER	1

Chain	Res	Type	Models (Total)
A	327	PRO	1
A	329	GLU	1
A	330	HIS	1
A	331	VAL	1
A	333	ARG	1
A	335	ILE	1
A	336	ALA	1
A	337	THR	1
A	338	ASN	1
A	340	THR	1
A	341	GLN	1
A	343	GLU	1
A	346	ILE	1
A	349	ASP	1
A	403	ASP	1
A	405	ASP	1
A	406	THR	1
A	408	LYS	1
A	409	ALA	1
A	410	GLU	1
A	413	VAL	1
A	414	SER	1
A	415	SER	1
A	416	VAL	1
A	417	LYS	1
A	418	VAL	1
A	419	VAL	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	348	304	19	25

There are 25 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	2	LEU	1
A	3	LEU	1
A	5	ILE	1
A	132	GLN	1
A	177	VAL	1
A	180	SER	1
A	210	VAL	1
A	213	LYS	1
A	240	GLU	1
A	279	VAL	1
A	280	ASN	1
A	286	GLU	1
A	289	LEU	1
A	291	GLU	1
A	293	ILE	1
A	315	THR	1
A	317	THR	1
A	320	THR	1
A	328	THR	1
A	332	ASP	1
A	340	THR	1
A	371	MET	1
A	374	LEU	1
A	405	ASP	1
A	415	SER	1

Fit of model to data used for modeling ?

Mass Spectrometry

Validation for this section is under development.

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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