Integrative Structure Validation Report

July 22, 2024 - 05:19 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	9A3G
PDB-Dev ID	PDBDEV_00000201
Structure Title	Invariant surface glycoprotein 65 of Trypanosoma brucei gambiense
Structure Authors	Suelzen, H.; Zoll, S.

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

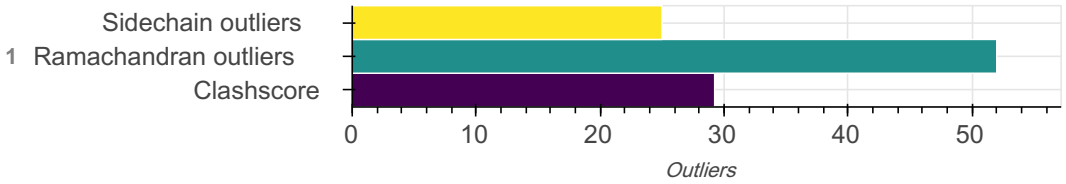
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 7 flexible or non-rigid units.

Entry composition

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Invariant surface glycoprotein 65	A	A	420

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

Representation

This entry has only one representation and includes 0 rigid bodies and 7 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-18, 19-129, 130-186, 187-210, 211-239, 240-296, 297-420

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	AlphaFold model prediction	None	None	False	False
2	1	None	Modelling	None	None	False	False
3	1	None	Refinement	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	Not available
2	Coot	Not available	model building	Not available
3	Phenix	Not available	refinement	Not available

Data quality

3DEM volume

Validation for this section is under development.

Mass Spectrometry

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 715 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA3	1.09	0.97	7
CG--HG3	1.09	0.97	26
CG2--HG21	1.09	0.97	14
NZ--HZ1	1.01	0.89	9
CB--HB3	1.09	0.97	74
CA--HA	1.09	0.97	88
CB--HB2	1.09	0.97	74
CA--HA2	1.09	0.97	7
CG1--HG13	1.09	0.97	9
CG2--HG23	1.09	0.97	14
CG1--HG12	1.09	0.97	9
CG2--HG22	1.09	0.97	14
CE--HE3	1.09	0.97	10
CD1--HD13	1.09	0.97	12
CB--HB	1.09	0.97	14
CG--HG2	1.09	0.97	26
CD--HD2	1.09	0.97	17
NZ--HZ3	1.01	0.89	9
CG--HG	1.09	0.97	7

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE--HE2	1.09	0.97	10
CD--HD3	1.09	0.97	17
OH--HH	0.96	0.84	3
CG1--HG11	1.09	0.97	4
CB--HB1	1.09	0.97	5
NZ--HZ2	1.01	0.89	9
CD1--HD11	1.09	0.97	12
CD2--HD23	1.09	0.97	7
OG--HG	0.96	0.84	10
CD2--HD21	1.09	0.97	7
OG1--HG1	0.96	0.84	5
CD1--HD12	1.09	0.97	12
CD2--HD22	1.09	0.97	7
CE--HE1	1.09	0.97	1
N--H	1.01	0.86	91
CD2--HD2	1.08	0.93	7
CZ--HZ	1.08	0.93	1
NE2--HE22	1.01	0.86	2
ND2--HD22	1.01	0.86	7
NH2--HH22	1.01	0.86	5
CE2--HE2	1.08	0.93	4
NH1--HH12	1.01	0.86	5
ND2--HD21	1.01	0.86	7

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND1--HD1	1.01	0.86	3
CE1--HE1	1.08	0.93	7
CD1--HD1	1.08	0.93	5
CZ2--HZ2	1.08	0.93	1
NH2--HH21	1.01	0.86	5
NE1--HE1	1.01	0.86	1
NE--HE	1.01	0.86	5
NH1--HH11	1.01	0.86	5
NE2--HE21	1.01	0.86	2
CZ3--HZ3	1.08	0.93	1
CE3--HE3	1.08	0.93	1
CH2--HH2	1.08	0.93	1

Standard geometry: angle outliers

There are 94 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
O-C-N	123.00	54.99	1
O-C-N	123.00	69.40	1
C-N-CA	121.70	91.17	1
C-N-CA	121.70	150.66	1
C-N-CA	121.70	149.13	1
C-N-CA	121.70	148.07	1
O-C-N	123.00	100.29	1
O-C-N	123.00	100.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	144.50	1
C-N-CA	121.70	143.41	1
C-N-CA	121.70	100.01	1
O-C-N	123.00	104.07	1
O-C-N	123.00	104.88	1
C-N-CA	121.70	141.89	1
O-C-N	123.00	105.24	1
C-N-CA	121.70	141.65	1
C-N-CA	121.70	141.57	1
C-N-CA	121.70	141.34	1
O-C-N	123.00	105.59	1
O-C-N	123.00	105.96	1
O-C-N	123.00	106.05	1
O-C-N	123.00	106.14	1
C-N-CA	121.70	140.54	1
O-C-N	123.00	106.53	1
O-C-N	123.00	106.86	1
C-N-CA	121.70	138.91	1
O-C-N	123.00	108.21	1
C-N-CA	121.70	138.25	1
C-N-CA	121.70	138.03	1
CA-N-CD	112.00	99.68	1
O-C-N	123.00	109.15	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	109.16	1
C-N-CA	121.70	137.15	1
C-N-CA	121.70	137.03	1
O-C-N	123.00	109.39	1
C-N-CA	121.70	136.62	1
O-C-N	123.00	109.85	1
O-C-N	123.00	110.03	1
C-N-CA	121.70	136.03	1
O-C-N	123.00	110.27	1
C-N-CA	121.70	135.92	1
O-C-N	123.00	110.50	1
C-N-CA	121.70	135.07	1
CA-C-N	116.20	130.44	1
C-N-CA	121.70	134.44	1
O-C-N	123.00	111.75	1
C-N-CA	121.70	134.35	1
O-C-N	123.00	112.03	1
O-C-N	123.00	112.15	1
O-C-N	123.00	112.31	1
O-C-N	123.00	112.58	1
O-C-N	123.00	112.76	1
O-C-N	123.00	112.78	1
C-N-CA	121.70	110.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	122.60	154.12	1
O-C-N	123.00	113.07	1
C-CA-CB	110.10	121.82	1
O-C-N	123.00	113.36	1
C-N-CA	121.70	111.31	1
C-N-CA	121.70	131.40	1
O-C-N	123.00	114.40	1
C-N-CD	125.00	103.12	1
C-N-CA	121.70	131.19	1
O-C-N	123.00	114.73	1
C-N-CA	121.70	112.41	1
C-N-CA	121.70	130.84	1
C-N-CA	121.70	130.70	1
CA-C-N	116.20	106.24	1
C-N-CD	125.00	104.67	1
C-N-CA	121.70	130.62	1
O-C-N	123.00	115.07	1
C-CA-CB	110.10	100.73	1
C-N-CA	121.70	112.93	1
CB-CG-CD2	131.20	124.93	1
O-C-N	123.00	115.48	1
O-C-N	123.00	115.52	1
O-C-N	123.00	115.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-CD	112.00	105.56	1
O-C-N	123.00	115.69	1
O-C-N	123.00	115.71	1
O-C-N	123.00	115.78	1
OE1-CD-NE2	122.60	118.15	1
CA-C-N	116.90	123.53	1
O-C-N	123.00	116.09	1
O-C-N	123.00	116.19	1
O-C-N	123.00	116.35	1
N-CA-CB	110.50	117.51	1
C-N-CA	121.70	129.11	1
O-C-N	123.00	116.41	1
O-C-N	123.00	116.42	1
NE-CZ-NH2	119.20	122.89	1
C-N-CA	121.70	129.04	1
CA-C-N	116.20	124.23	1
C-N-H	109.92	124.30	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	29.24	190

All 190 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:144:LEU:CG	A:245:TYR:OH	1.407
1	A:96:LYS:NZ	A:348:ALA:CB	1.382
1	A:144:LEU:CD1	A:245:TYR:OH	1.345
1	A:20:LYS:HG3	A:166:ASP:O	1.261
1	A:302:LYS:CA	A:303:GLY:N	1.250
1	A:18:LEU:C	A:19:THR:N	1.219
1	A:293:ILE:HD11	A:354:LEU:CD2	1.215
1	A:293:ILE:CD1	A:354:LEU:CD2	1.207
1	A:96:LYS:NZ	A:348:ALA:HB1	1.186
1	A:146:ARG:HB2	A:241:TRP:CZ2	1.185
1	A:23:ALA:HB2	A:168:ILE:CD1	1.182
1	A:293:ILE:CD1	A:354:LEU:HD23	1.169
1	A:418:VAL:O	A:419:VAL:HG23	1.166
1	A:186:SER:O	A:187:THR:HG23	1.158
1	A:96:LYS:NZ	A:348:ALA:HB2	1.155
1	A:336:ALA:O	A:337:THR:HG23	1.141
1	A:144:LEU:HG	A:245:TYR:OH	1.139
1	A:315:THR:HG22	A:316:PRO:HD3	1.135
1	A:20:LYS:HA	A:168:ILE:HG13	1.132
1	A:19:THR:HA	A:166:ASP:HB3	1.127
1	A:315:THR:HG22	A:316:PRO:CD	1.114
1	A:334:GLY:O	A:335:ILE:HG13	1.108
1	A:23:ALA:CB	A:168:ILE:HD13	1.104

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:20:LYS:CG	A:166:ASP:O	1.098
1	A:315:THR:CG2	A:316:PRO:HD3	1.097
1	A:20:LYS:N	A:166:ASP:O	1.085
1	A:293:ILE:HG13	A:354:LEU:HD22	1.080
1	A:297:LYS:HE3	A:354:LEU:HB3	1.075
1	A:146:ARG:HB2	A:241:TRP:CH2	1.058
1	A:18:LEU:HD12	A:22:GLY:HA3	1.053
1	A:144:LEU:HD12	A:245:TYR:OH	1.049
1	A:144:LEU:HD11	A:245:TYR:CE2	1.046
1	A:18:LEU:CD1	A:22:GLY:HA3	1.034
1	A:96:LYS:HZ2	A:348:ALA:HB1	1.025
1	A:30:LYS:HE2	A:144:LEU:O	1.020
1	A:293:ILE:CG1	A:354:LEU:HD22	1.020
1	A:293:ILE:HD11	A:354:LEU:HD23	1.019
1	A:23:ALA:CB	A:168:ILE:CD1	1.008
1	A:27:CYS:SG	A:182:ILE:HG22	1.005
1	A:293:ILE:CD1	A:354:LEU:HD22	1.004
1	A:18:LEU:O	A:19:THR:N	1.003
1	A:20:LYS:HA	A:168:ILE:CG1	0.999
1	A:144:LEU:CD1	A:245:TYR:CZ	0.997
1	A:20:LYS:HG3	A:166:ASP:C	0.994
1	A:144:LEU:HG	A:245:TYR:CZ	0.989
1	A:23:ALA:HB2	A:168:ILE:HD13	0.966

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:146:ARG:CB	A:241:TRP:CH2	0.951
1	A:96:LYS:HZ3	A:348:ALA:CB	0.928
1	A:186:SER:O	A:187:THR:CG2	0.926
1	A:30:LYS:CE	A:144:LEU:O	0.924
1	A:96:LYS:HZ1	A:348:ALA:HB2	0.919
1	A:297:LYS:CE	A:354:LEU:HB3	0.913
1	A:297:LYS:HG3	A:354:LEU:HD13	0.911
1	A:297:LYS:CG	A:354:LEU:HD13	0.905
1	A:96:LYS:HZ1	A:348:ALA:CB	0.879
1	A:336:ALA:C	A:337:THR:HG23	0.874
1	A:302:LYS:C	A:303:GLY:N	0.860
1	A:92:GLU:OE2	A:350:PHE:CZ	0.844
1	A:18:LEU:HD11	A:22:GLY:C	0.840
1	A:23:ALA:HB3	A:168:ILE:HG12	0.840
1	A:30:LYS:HG2	A:144:LEU:HB3	0.830
1	A:334:GLY:C	A:335:ILE:HG13	0.829
1	A:327:PRO:O	A:328:THR:HG23	0.817
1	A:26:LEU:HG	A:148:LEU:HD21	0.811
1	A:144:LEU:CD1	A:245:TYR:CE2	0.811
1	A:27:CYS:SG	A:182:ILE:CG2	0.808
1	A:129:ALA:HA	A:131:GLY:N	0.803
1	A:144:LEU:HD11	A:245:TYR:CZ	0.797
1	A:418:VAL:C	A:419:VAL:HG23	0.797

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:26:LEU:HG	A:148:LEU:CD2	0.793
1	A:18:LEU:CD1	A:22:GLY:CA	0.786
1	A:20:LYS:CA	A:168:ILE:HG13	0.773
1	A:96:LYS:HZ3	A:348:ALA:HB2	0.769
1	A:289:LEU:HB2	A:361:GLU:OE2	0.764
1	A:409:ALA:HB1	A:410:GLU:HG3	0.764
1	A:144:LEU:CG	A:245:TYR:CZ	0.751
1	A:203:ALA:O	A:206:SER:OG	0.747
1	A:145:TYR:N	A:241:TRP:CZ3	0.736
1	A:336:ALA:O	A:337:THR:CG2	0.721
1	A:418:VAL:O	A:419:VAL:CG2	0.714
1	A:146:ARG:CB	A:241:TRP:CZ2	0.709
1	A:293:ILE:HD12	A:354:LEU:CD2	0.708
1	A:23:ALA:HB3	A:168:ILE:CG1	0.706
1	A:20:LYS:CA	A:166:ASP:O	0.692
1	A:17:LYS:C	A:19:THR:N	0.686
1	A:297:LYS:CE	A:354:LEU:CB	0.682
1	A:194:ASP:OD1	A:196:SER:OG	0.681
1	A:315:THR:HG22	A:316:PRO:HD2	0.670
1	A:30:LYS:HE2	A:144:LEU:C	0.667
1	A:186:SER:C	A:187:THR:HG23	0.661
1	A:373:ILE:CG2	A:377:LEU:HD12	0.659
1	A:19:THR:OG1	A:21:GLU:OE1	0.658

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:86:ASP:OD1	A:289:LEU:HB3	0.640
1	A:402:HIS:O	A:403:ASP:HB2	0.640
1	A:85:SER:OG	A:89:LYS:NZ	0.640
1	A:144:LEU:HD11	A:245:TYR:HE2	0.638
1	A:18:LEU:CD1	A:22:GLY:C	0.637
1	A:297:LYS:HG2	A:354:LEU:HD13	0.635
1	A:18:LEU:HD11	A:22:GLY:CA	0.631
1	A:23:ALA:HB3	A:168:ILE:CD1	0.631
1	A:297:LYS:HE2	A:354:LEU:CB	0.631
1	A:145:TYR:N	A:241:TRP:HZ3	0.620
1	A:144:LEU:CG	A:245:TYR:CE2	0.617
1	A:306:ILE:HG22	A:308:ILE:HG13	0.617
1	A:378:VAL:HB	A:379:PRO:HD3	0.608
1	A:315:THR:CG2	A:316:PRO:CD	0.606
1	A:96:LYS:HZ2	A:350:PHE:HE2	0.600
1	A:336:ALA:C	A:337:THR:CG2	0.597
1	A:418:VAL:C	A:419:VAL:CG2	0.597
1	A:297:LYS:HE2	A:354:LEU:HB2	0.596
1	A:209:ASP:O	A:210:VAL:C	0.591
1	A:96:LYS:NZ	A:350:PHE:HE2	0.589
1	A:20:LYS:CB	A:166:ASP:O	0.589
1	A:18:LEU:HG	A:23:ALA:N	0.583
1	A:373:ILE:HG22	A:377:LEU:HD12	0.581

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:23:ALA:CB	A:168:ILE:CG1	0.579
1	A:209:ASP:HA	A:211:LYS:HB3	0.577
1	A:405:ASP:HB3	A:406:THR:HG23	0.576
1	A:26:LEU:HD23	A:148:LEU:HD23	0.575
1	A:334:GLY:C	A:335:ILE:CG1	0.574
1	A:293:ILE:HD11	A:354:LEU:HA	0.572
1	A:19:THR:HA	A:166:ASP:CB	0.567
1	A:297:LYS:HG2	A:354:LEU:CD1	0.566
1	A:302:LYS:N	A:303:GLY:N	0.566
1	A:26:LEU:CD2	A:147:VAL:HG12	0.561
1	A:139:ALA:HB1	A:179:ARG:HH12	0.555
1	A:239:GLU:HA	A:242:GLN:HB2	0.549
1	A:146:ARG:HB3	A:241:TRP:CE3	0.548
1	A:144:LEU:C	A:241:TRP:CZ3	0.545
1	A:354:LEU:O	A:357:THR:OG1	0.538
1	A:30:LYS:CG	A:144:LEU:HB3	0.536
1	A:26:LEU:CD2	A:148:LEU:HD23	0.531
1	A:20:LYS:CG	A:166:ASP:C	0.531
1	A:280:ASN:HD22	A:281:THR:N	0.531
1	A:153:ILE:CD1	A:180:SER:HB2	0.530
1	A:129:ALA:HA	A:130:ARG:C	0.529
1	A:143:GLY:HA2	A:241:TRP:HB3	0.528
1	A:402:HIS:O	A:403:ASP:CB	0.523

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:58:GLU:OE1	A:273:ALA:HB1	0.522
1	A:144:LEU:CB	A:245:TYR:OH	0.518
1	A:118:LEU:HD22	A:255:LEU:HB2	0.512
1	A:415:SER:HA	A:416:VAL:HG23	0.512
1	A:96:LYS:HD2	A:350:PHE:CZ	0.510
1	A:144:LEU:HD21	A:245:TYR:HE2	0.510
1	A:26:LEU:HD22	A:147:VAL:HG12	0.506
1	A:146:ARG:HB2	A:241:TRP:CE2	0.505
1	A:373:ILE:HG23	A:377:LEU:HD12	0.497
1	A:18:LEU:HD21	A:23:ALA:HA	0.491
1	A:280:ASN:C	A:280:ASN:ND2	0.491
1	A:30:LYS:HE3	A:144:LEU:O	0.486
1	A:18:LEU:O	A:19:THR:CA	0.484
1	A:203:ALA:O	A:207:TRP:CE3	0.479
1	A:348:ALA:HB1	A:350:PHE:CE2	0.475
1	A:143:GLY:HA2	A:241:TRP:CB	0.473
1	A:170:PHE:CG	A:180:SER:HB3	0.472
1	A:315:THR:CB	A:316:PRO:CD	0.472
1	A:249:VAL:HG22	A:253:ARG:HE	0.468
1	A:26:LEU:CG	A:148:LEU:CD2	0.466
1	A:20:LYS:HG2	A:168:ILE:HG13	0.465
1	A:144:LEU:C	A:241:TRP:HZ3	0.465
1	A:374:LEU:O	A:378:VAL:HG23	0.465

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:419:VAL:HG12	A:420:MET:HB2	0.465
1	A:15:ASP:OD1	A:212:PRO:HA	0.464
1	A:280:ASN:C	A:280:ASN:HD22	0.461
1	A:27:CYS:SG	A:182:ILE:HG21	0.459
1	A:412:GLY:CA	A:413:VAL:HG23	0.458
1	A:203:ALA:HB1	A:207:TRP:CZ3	0.457
1	A:129:ALA:CA	A:131:GLY:N	0.454
1	A:211:LYS:HE3	A:213:LYS:HA	0.450
1	A:329:GLU:O	A:330:HIS:CD2	0.445
1	A:26:LEU:HD21	A:147:VAL:HG12	0.437
1	A:358:GLU:O	A:362:VAL:HG23	0.436
1	A:208:GLU:O	A:211:LYS:HB3	0.434
1	A:329:GLU:O	A:330:HIS:CG	0.432
1	A:18:LEU:HB2	A:151:TYR:CE1	0.429
1	A:18:LEU:N	A:19:THR:N	0.428
1	A:146:ARG:CB	A:241:TRP:CE2	0.425
1	A:143:GLY:C	A:241:TRP:CB	0.425
1	A:27:CYS:HB3	A:184:CYS:HB3	0.424
1	A:96:LYS:HD2	A:350:PHE:CE2	0.423
1	A:129:ALA:HB3	A:244:PRO:HG3	0.416
1	A:186:SER:C	A:187:THR:CB	0.415
1	A:208:GLU:O	A:211:LYS:N	0.414
1	A:378:VAL:N	A:379:PRO:CD	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:416:VAL:O	A:417:LYS:HB2	0.408
1	A:89:LYS:HG2	A:293:ILE:CD1	0.406
1	A:20:LYS:HA	A:168:ILE:CD1	0.404
1	A:37:ALA:O	A:41:SER:OG	0.404
1	A:98:LYS:O	A:102:THR:HG23	0.401
1	A:243:THR:N	A:244:PRO:HD2	0.400

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	Analyzed	Favored	Allowed	Outliers
1	418	322	44	52

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	Analyzed	Favored	Allowed	Outliers
1	348	304	19	25

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	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

Model ID	Chain	Residue ID	Residue type
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

Fit of model to data used for modeling

3DEM volume

Validation for this section is under development.

Mass Spectrometry

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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