Integrative Structure Validation Report

July 22, 2024 - 04:47 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	9A20
PDB-Dev ID	PDBDEV_00000132
Structure Title	NMR Structure of Sa1_V90T at 5 Degrees Celsius
Structure Authors	Solomon, T.L.; Orban, J.

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

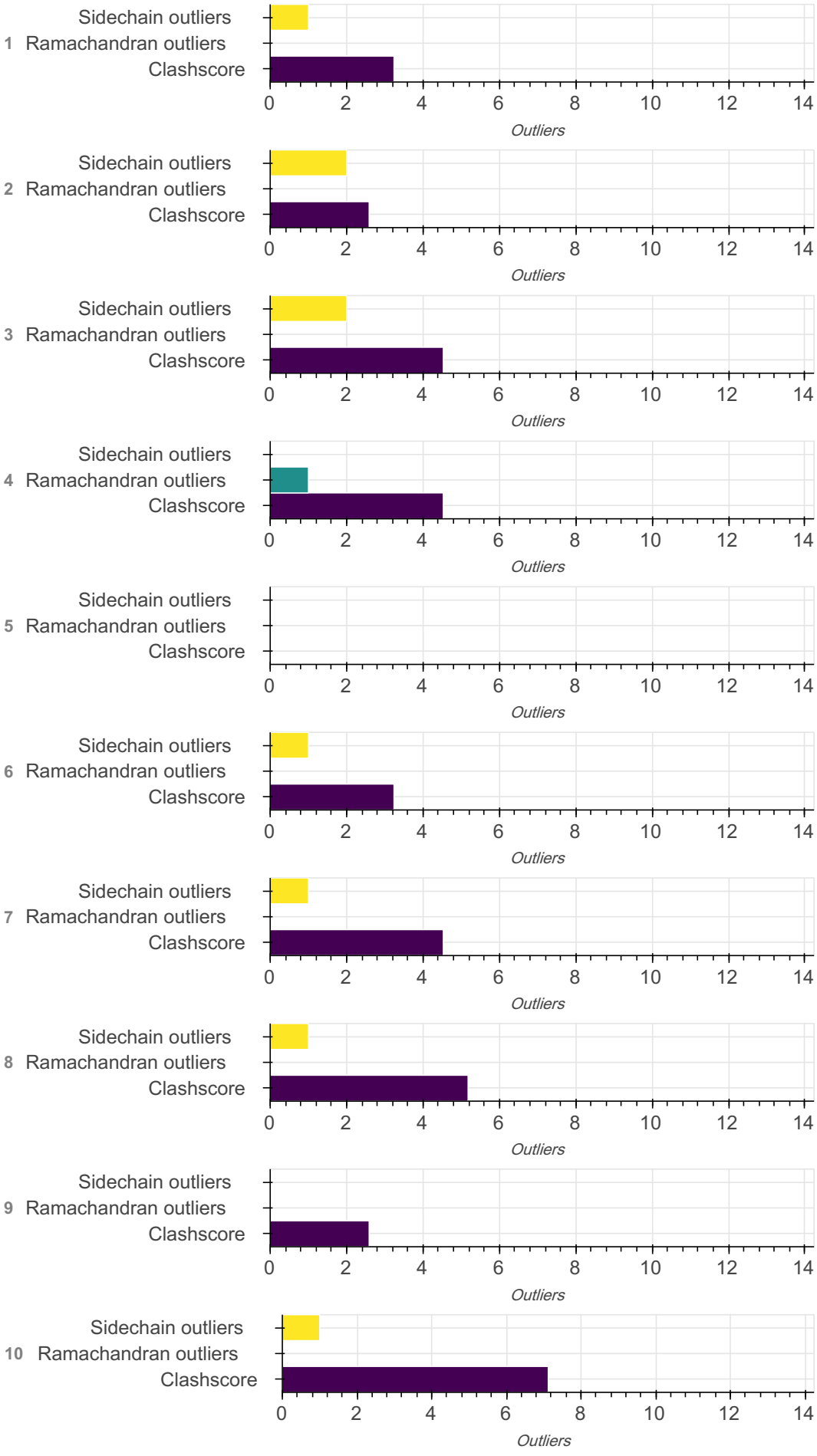
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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


1
2
3
4
5
6
7
8
9
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
2
4
6
8
10
12
14
Outliers

Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 10 unique models, with 1 subunits in each model. A total of 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.

Entry composition

There are 10 unique types of models in this entry.These models are titled None, None, None, None, None, None, None, None, None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95
2	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95
3	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95
4	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95
5	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95
6	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95
7	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95
8	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95
9	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	1	1	3-alpha NMR structure of Sa1_V90T at 5 degrees Celsius	A	A	95

Datasets used for modeling

There is 1 unique dataset used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	NMR data	BMRB	51338

Representation

This entry has only one representation and includes 0 rigid bodies and 1 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-95

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 is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	CS-Rosetta	Not available	model building	https://pubmed.ncbi.nlm.nih.gov/18326625/

Data quality

NMR

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 7990 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
N--H1	1.00	0.89	10
N--H2	1.00	0.89	10
N--H3	1.00	0.89	10
CB--HB3	1.09	0.97	680
CB--HB2	1.09	0.97	680
CG--HG3	1.09	0.97	290
CD1--HD13	1.09	0.97	200
CG2--HG23	1.09	0.97	210
CG--HG2	1.09	0.97	290
CG2--HG22	1.09	0.97	210
CE--HE2	1.09	0.97	100
CD--HD3	1.09	0.97	150
NZ--HZ3	1.01	0.89	100
CG2--HG21	1.09	0.97	210
CA--HA3	1.09	0.97	40
CB--HB	1.09	0.97	210

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.09	0.97	890
CG1--HG12	1.09	0.97	170
CD1--HD12	1.09	0.97	200
CD--HD2	1.09	0.97	150
CD1--HD11	1.09	0.97	200
CG--HG	1.09	0.97	120
OG1--HG1	0.96	0.84	40
CD2--HD23	1.09	0.97	120
CD2--HD21	1.09	0.97	120
CG1--HG13	1.09	0.97	170
CB--HB1	1.09	0.97	120
CE--HE3	1.09	0.97	100
OH--HH	0.96	0.84	30
CD2--HD22	1.09	0.97	120
NZ--HZ1	1.01	0.89	100
CG1--HG11	1.09	0.97	90
CA--HA2	1.09	0.97	40
OG--HG	0.96	0.84	10
NZ--HZ2	1.01	0.89	100
CG--HG3	1.10	0.97	20
CB--HB3	1.10	0.97	20
CA--HA	1.10	0.97	20
CG--HG2	1.10	0.97	20

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD--HD3	1.10	0.97	20
CD--HD2	1.10	0.97	20
CB--HB2	1.10	0.97	20
ND2--HD22	1.00	0.86	50
NE2--HE22	1.00	0.86	60
ND2--HD21	1.00	0.86	50
NE2--HE21	1.00	0.86	60
NH2--HH22	1.01	0.86	50
NH1--HH12	1.01	0.86	50
N--H	1.01	0.86	920
NH1--HH11	1.01	0.86	50
NH2--HH21	1.01	0.86	50
NE--HE	1.01	0.86	50
CZ--HZ	1.09	0.93	10
CD1--HD1	1.09	0.93	40
CD2--HD2	1.09	0.93	40
CE1--HE1	1.09	0.93	40
CE2--HE2	1.09	0.93	40

Standard geometry: angle outliers

There are 250 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
CZ-NE-HE	105.90	117.90	1
CZ-NE-HE	105.89	117.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CZ-NE-HE	105.88	117.90	3
CZ-NE-HE	105.87	117.90	1
CZ-NE-HE	105.86	117.90	1
CZ-NE-HE	105.85	117.90	4
CZ-NE-HE	105.84	117.90	2
CZ-NE-HE	105.83	117.90	3
CZ-NE-HE	105.82	117.90	5
CZ-NE-HE	105.81	117.90	4
CZ-NE-HE	105.80	117.90	5
CZ-NE-HE	105.79	117.90	3
CZ-NE-HE	105.78	117.90	6
CZ-NE-HE	105.77	117.90	5
CZ-NE-HE	105.75	117.90	3
CZ-NE-HE	105.73	117.90	2
CZ-NE-HE	105.70	117.90	1
H2-N-H3	97.24	109.47	1
H1-N-H2	97.23	109.47	1
H2-N-H3	97.21	109.47	1
H1-N-H3	97.20	109.47	1
H1-N-H3	97.19	109.47	3
H2-N-H3	97.19	109.47	1
H1-N-H2	97.19	109.47	1
H1-N-H3	97.18	109.47	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H1-N-H2	97.18	109.47	2
H2-N-H3	97.18	109.47	2
H1-N-H2	97.17	109.47	2
H1-N-H2	97.16	109.47	2
H2-N-H3	97.16	109.47	1
H1-N-H3	97.16	109.47	2
H1-N-H2	97.15	109.47	1
H2-N-H3	97.15	109.47	2
H1-N-H3	97.14	109.47	1
H1-N-H2	97.14	109.47	1
H2-N-H3	97.13	109.47	1
H1-N-H3	97.13	109.47	1
H2-N-H3	97.11	109.47	1
CB-CG-HG2	122.71	109.00	1
CB-CG-HG2	122.72	109.00	4
CB-CG-HG2	122.73	109.00	3
CB-CG-HG2	122.74	109.00	3
CB-CG-HG2	122.75	109.00	7
CB-CG-HG2	122.76	109.00	5
CB-CG-HG2	122.77	109.00	7
CB-CG-HG2	122.78	109.00	7
CB-CG-HG2	122.79	109.00	8
CB-CG-HG2	122.80	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-HG2	122.81	109.00	2
CB-CG-HG2	122.82	109.00	3
CB-CG-HG2	122.83	109.00	4
CB-CG-HG2	122.84	109.00	1
CB-CG-HG2	122.85	109.00	2
CB-CG-HG3	94.65	109.00	1
CB-CG-HG3	94.62	109.00	1
CB-CG-HG3	94.61	109.00	1
CB-CG-HG3	94.60	109.00	2
CB-CG-HG3	94.59	109.00	3
CB-CG-HG3	94.58	109.00	8
CB-CG-HG3	94.57	109.00	6
CB-CG-HG3	94.56	109.00	4
CB-CG-HG3	94.55	109.00	5
CB-CG-HG3	94.54	109.00	5
CB-CG-HG3	94.53	109.00	9
CB-CG-HG3	94.52	109.00	7
CB-CG-HG3	94.51	109.00	5
CB-CG-HG3	94.49	109.00	1
CB-CG-HG3	94.48	109.00	1
CB-CG-HG3	94.47	109.00	1
CA-CB-HB3	93.41	109.00	1
CA-CB-HB3	93.39	109.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB3	93.38	109.00	2
CA-CB-HB3	93.37	109.00	3
CA-CB-HB3	93.36	109.00	4
CA-CB-HB3	93.35	109.00	5
CA-CB-HB3	93.34	109.00	4
CA-CB-HB3	93.33	109.00	13
CA-CB-HB3	93.32	109.00	5
CA-CB-HB3	93.31	109.00	4
CA-CB-HB3	93.30	109.00	1
CA-CB-HB3	93.29	109.00	1
CA-CB-HB3	93.28	109.00	1
CA-CB-HB3	93.27	109.00	2
CA-CB-HB3	93.26	109.00	1
CA-CB-HB3	93.23	109.00	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	3.24	5
2	2.59	4
3	4.53	7
4	4.53	7
5	0.00	0

Model ID	Clash score	Number of clashes
6	3.24	5
7	4.53	7
8	5.18	8
9	2.59	4
10	7.12	11

All 58 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:11:ASN:HB2	A:12:PRO:HD2	0.631
1	A:95:ASP:OD1	A:95:ASP:OXT	0.564
1	A:61:LEU:O	A:64:GLN:HG2	0.490
1	A:82:LEU:HG	A:82:LEU:O	0.448
1	A:68:PRO:HB2	A:71:ARG:CG	0.413
2	A:8:ILE:HG13	A:10:LEU:CD1	0.511
2	A:67:ALA:HB1	A:68:PRO:HD2	0.484
2	A:8:ILE:HG13	A:10:LEU:HD12	0.465
2	A:11:ASN:HA	A:12:PRO:HD2	0.404
3	A:63:TYR:O	A:64:GLN:C	0.635
3	A:65:ILE:H	A:65:ILE:HD13	0.622
3	A:65:ILE:N	A:65:ILE:HD13	0.587
3	A:85:VAL:O	A:85:VAL:HG12	0.473
3	A:3:THR:HG21	A:45:ASN:HB3	0.441
3	A:39:LYS:HD2	A:39:LYS:N	0.437
3	A:11:ASN:N	A:12:PRO:HD3	0.407

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:11:ASN:HB2	A:12:PRO:HD2	0.617
4	A:75:LEU:C	A:75:LEU:HD23	0.602
4	A:8:ILE:HG22	A:10:LEU:H	0.584
4	A:10:LEU:C	A:10:LEU:HD23	0.539
4	A:82:LEU:HG	A:84:ALA:H	0.531
4	A:67:ALA:HB1	A:68:PRO:HD2	0.479
4	A:75:LEU:C	A:75:LEU:CD2	0.415
6	A:6:VAL:HG23	A:8:ILE:HG12	0.494
6	A:6:VAL:O	A:6:VAL:HG22	0.484
6	A:85:VAL:O	A:85:VAL:HG12	0.476
6	A:65:ILE:O	A:65:ILE:HG22	0.473
6	A:5:GLU:HG2	A:5:GLU:O	0.436
7	A:11:ASN:HB2	A:12:PRO:CD	0.705
7	A:11:ASN:HB2	A:12:PRO:HD2	0.674
7	A:8:ILE:C	A:8:ILE:HD12	0.565
7	A:82:LEU:O	A:82:LEU:HD23	0.544
7	A:67:ALA:HB1	A:68:PRO:HD2	0.434
7	A:11:ASN:CB	A:12:PRO:CD	0.422
7	A:82:LEU:C	A:82:LEU:HD23	0.401
8	A:67:ALA:HB1	A:68:PRO:CD	0.552
8	A:11:ASN:CB	A:14:LEU:HB2	0.525
8	A:63:TYR:O	A:64:GLN:C	0.524
8	A:64:GLN:HB3	A:67:ALA:CB	0.522

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:11:ASN:HB3	A:14:LEU:HB2	0.516
8	A:64:GLN:HB3	A:67:ALA:HB3	0.482
8	A:67:ALA:HB1	A:68:PRO:HD2	0.470
8	A:65:ILE:HG22	A:66:GLU:N	0.420
9	A:65:ILE:O	A:65:ILE:HG22	0.839
9	A:95:ASP:OD1	A:95:ASP:OXT	0.634
9	A:65:ILE:CG2	A:65:ILE:O	0.608
9	A:85:VAL:O	A:85:VAL:HG12	0.518
10	A:8:ILE:CD1	A:8:ILE:N	1.102
10	A:8:ILE:H	A:8:ILE:HD13	1.082
10	A:8:ILE:CD1	A:8:ILE:H	0.990
10	A:8:ILE:N	A:8:ILE:HD13	0.929
10	A:8:ILE:N	A:8:ILE:HD12	0.847
10	A:85:VAL:O	A:85:VAL:HG12	0.588
10	A:71:ARG:HG2	A:71:ARG:O	0.497
10	A:64:GLN:HG2	A:66:GLU:H	0.485
10	A:65:ILE:HG13	A:66:GLU:HG2	0.458
10	A:85:VAL:CG1	A:85:VAL:O	0.456
10	A:64:GLN:HB3	A:67:ALA:HB3	0.434

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	93	92	1	0

Model ID	Analyzed	Favored	Allowed	Outliers
2	93	93	0	0
3	93	92	1	0
4	93	90	2	1
5	93	89	4	0
6	93	91	2	0
7	93	91	2	0
8	93	90	3	0
9	93	90	3	0
10	93	89	4	0

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	79	78	0	1
2	79	76	1	2
3	79	76	1	2
4	79	77	2	0
5	79	79	0	0
6	79	78	0	1
7	79	76	2	1
8	79	78	0	1
9	79	79	0	0
10	79	76	2	1

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	91	THR
2	A	30	LEU
2	A	88	VAL
3	A	65	ILE
3	A	73	ASN
6	A	6	VAL
7	A	6	VAL
8	A	65	ILE
10	A	8	ILE

Fit of model to data used for modeling

NMR

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 labcontributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded byRCSB PDB (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from RCSB PDB, Dr. Jill Trewhella, 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.