# Integrative Structure Validation Report July 22, 2024 - 05:38 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	9A83			
PDB-Dev ID	PDBDEV_00000368			
Structure Title	Encounter complex in the cross-modular condensation step of the Tomaymycin NRPS system: complex of the substrate-loaded peptidyl-carrier-protein domain from the TomA module (APCP- load) with the adaptor (BN91) of the TomB module			
Structure Authors	Karanth, M.N.; Kirkpatrick, J. P.; Carlomagno, T.			

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 o

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 1 distinct ensemble(s).

#### Summary ?

This entry consists of 10 unique models, with 2 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 2 flexible or non-rigid units.

### Entry composition?

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73
1	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module		В	72
2	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73
2	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72
3	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73
3	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72
4	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72
5	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73
5	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72
6	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73
6	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72
7	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73
7	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72
8	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73
8	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72
9	1	1	Adaptor BN91 domain of Tomaymycin B module	A	A	73
9	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72
10	1	1	Adaptor BN91 domain of Tomaymycin B module	А	A	73

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	2	2	Substrate-loaded form of the peptidyl-carrier- protein (APCP) domain of the Tomaymycin A module	В	В	72

# Datasets used for modeling @

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	NMR data	Not available	Not available
2	Experimental model	PDB	8QSX
3	Experimental model	PDB	8QRX

### Representation ?

This entry has only one representation and includes 0 rigid bodies and 2 flexible units

Chain ID	Rigid bodies	Non-rigid segments
В	-	1-72
А	-	1-73

## 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
----------------	----------------	-------------	----------------	-----------------------	------------------------------------	----------------------------	----------------------------

#### 6 of 34

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Data-driven docking using CSP-derived distance restraints within HADDOCK.	None	Data-driven docking using CSP-derived distance restraints within HADDOCK.	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.4	Data-driven docking	https://wenmr.science.uu.nl/haddock2.4/



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 2380 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Bond type Observed distance (Å)		Number of outliers
NE2HE22 0.97		0.86	7
NH	0.97	0.86	27
ND2HD22	0.97	0.86	1
NH	0.98	0.86	1331
OG1HG1 0.96		0.84	67

7 of 34

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
ND2HD21	0.98	0.86	10
ND2HD22	0.98	0.86	19
NE2HE22	0.98	0.86	43
NE2HE21	0.98	0.86	41
ND1HD1	0.98	0.86	19
NE2HE2	0.98	0.86	24
NEHE	0.98	0.86	68
OGHG	0.96	0.84	55
NE1HE1	0.98	0.86	10
SGHG	1.32	1.20	8
NEHE	0.99	0.86	22
NH	0.99	0.86	32
SGHG	1.33	1.20	2
OG1HG1	0.97	0.84	79
OGHG	0.97	0.84	14
NE2HE2	0.99	0.86	15
NE2HE21	0.99	0.86	8
ND2HD21	0.99	0.86	8
ND1HD1	0.99	0.86	19
ND2HD21	1.00	0.86	2
OG1HG1	0.98	0.84	14
NE2HE2	1.00	0.86	1
OGHG	0.98	0.84	11

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
ND1HD1	1.00	0.86	2
NE2HE21	1.00	0.86	1
NZHZ3	1.04	0.89	3
NZHZ2	1.04	0.89	20
NZHZ1	1.04	0.89	19
NZHZ3	1.05	0.89	17
NZHZ1	1.05	0.89	1
NH1HH11	1.03	0.86	1
NH1HH12	1.03	0.86	2
NH1HH11	1.04	0.86	72
NH1HH12	1.04	0.86	49
NH2HH22	1.04	0.86	44
NH2HH21	1.04	0.86	60
NH2HH22	1.05	0.86	37
NH1HH11	1.05	0.86	11
NH1HH12	1.05	0.86	12
NH2HH21	1.05	0.86	18
NH1HH12	1.06	0.86	27
NH2HH21	1.06	0.86	12
NH2HH22	1.06	0.86	9
NH1HH11	1.06	0.86	6

Standard geometry: angle outliers?

Bond angle outliers do not exist or can not be evaluated for this model

Too-close contacts?

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of

IM Structure Validation Report

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	14.79	32
2	14.79	32
3	16.64	36
4	18.02	39
5	15.71	34
6	19.87	43
7	16.64	36
8	14.33	31
9	16.64	36
10	16.17	35

All 354 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:6:THR:HG21	B:6:VAL:HG21	0.726
1	A:2:PRO:HG2	B:3:LEU:HD13	0.665
1	A:3:LEU:HD21	B:3:LEU:HA	0.656
1	B:12:LYS:HZ2	B:18:ASP:HA	0.651
1	A:43:LEU:HA	A:46:VAL:HG12	0.607
1	B:3:LEU:HD23	B:66:ALA:HA	0.577
1	A:6:THR:HB	A:47:PHE:HZ	0.570
1	B:12:LYS:NZ	B:18:ASP:HA	0.543
1	A:32:HIS:O	A:35:LEU:HG	0.528
1	A:51:ILE:HD12	A:68:ARG:HD3	0.527

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:54:GLU:O	B:58:ARG:HG3	0.518
1	B:32:ASN:HB3	B:35:HIS:HB2	0.506
1	B:3:LEU:O	B:7:VAL:HG23	0.505
1	B:39:LEU:O	B:43:LEU:HG	0.505
1	A:44:THR:HG22	A:50:GLU:HG2	0.501
1	B:41:SER:HA	B:44:GLN:HG3	0.499
1	B:44:GLN:HG2	B:51:VAL:H	0.489
1	A:3:LEU:HD23	B:3:LEU:HD12	0.478
1	A:22:ALA:HA	A:62:VAL:HG22	0.477
1	B:63:GLU:OE2	B:64:GLN:HG2	0.476
1	B:3:LEU:HB3	B:66:ALA:HB1	0.475
1	A:10:LEU:HD11	A:43:LEU:HD21	0.460
1	B:1:ASN:O	B:4:GLU:HB2	0.460
1	A:6:THR:HB	A:47:PHE:CZ	0.459
1	B:20:PHE:HZ	B:62:VAL:HG13	0.449
1	A:3:LEU:HD22	A:47:PHE:CE2	0.448
1	B:12:LYS:O	B:16:GLY:HA2	0.437
1	B:24:ASP:O	B:61:THR:HA	0.433
1	A:3:LEU:O	A:7:VAL:HG23	0.429
1	A:39:LEU:HD23	A:56:LEU:HD21	0.426
1	B:45:LYS:HB2	B:45:LYS:HE3	0.418
1	A:5:THR:HG21	B:48:GLY:HA2	0.403
2	A:6:THR:HG23	B:46:ILE:HB	0.896

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:6:THR:HG21	B:6:VAL:HG21	0.819
2	A:43:LEU:HA	A:46:VAL:HG12	0.724
2	B:12:LYS:HZ2	B:18:ASP:HA	0.616
2	A:3:LEU:HD21	B:3:LEU:HA	0.586
2	A:46:VAL:HG22	B:6:VAL:HG23	0.565
2	B:12:LYS:NZ	B:18:ASP:HA	0.535
2	A:3:LEU:O	A:7:VAL:HG23	0.524
2	A:32:HIS:O	A:35:LEU:HG	0.503
2	A:47:PHE:C	B:5:THR:HG21	0.500
2	B:3:LEU:HD23	B:66:ALA:HA	0.498
2	A:3:LEU:HD22	A:47:PHE:CE2	0.477
2	B:39:LEU:O	B:43:LEU:HG	0.477
2	A:39:LEU:O	A:43:LEU:HG	0.474
2	A:3:LEU:HA	A:6:THR:OG1	0.473
2	A:11:ALA:O	A:15:LEU:HB2	0.472
2	B:3:LEU:O	B:7:VAL:HG23	0.458
2	A:61:THR:H	A:64:ASP:HB3	0.451
2	B:32:ASN:HB3	B:35:HIS:HB2	0.450
2	B:12:LYS:O	B:16:GLY:HA2	0.443
2	B:22:THR:O	B:62:VAL:HG22	0.442
2	B:8:LEU:CD1	B:12:LYS:HE2	0.437
2	B:44:GLN:HG2	B:51:VAL:H	0.435
2	B:53:THR:HA	B:56:VAL:HG22	0.428

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:2:PRO:O	B:5:THR:HG22	0.422
2	B:56:VAL:HG12	B:65:LEU:HD21	0.421
2	A:46:VAL:HG23	B:9:GLN:HG3	0.417
2	B:7:VAL:HG21	B:66:ALA:HB2	0.416
2	A:26:LEU:O	A:30:CYS:HB2	0.414
2	B:40:ALA:O	B:44:GLN:HG3	0.413
2	A:21:THR:HG22	A:22:ALA:H	0.410
2	B:22:THR:C	B:24:ASP:H	0.402
3	B:9:GLN:HA	B:12:LYS:HD2	0.964
3	A:73:ARG:HE	B:70:GLU:HB3	0.812
3	A:6:THR:HB	A:47:PHE:HZ	0.807
3	B:12:LYS:HG2	B:18:ASP:HA	0.791
3	A:43:LEU:HA	A:46:VAL:HG12	0.756
3	B:56:VAL:HA	B:65:LEU:HD21	0.701
3	A:4:ARG:HE	A:63:ALA:HA	0.654
3	B:9:GLN:HA	B:12:LYS:CD	0.641
3	B:47:PHE:HD1	B:51:VAL:HG21	0.574
3	A:1:SER:N	A:4:ARG:HH12	0.563
3	A:6:THR:HB	A:47:PHE:CZ	0.562
3	A:73:ARG:NE	B:70:GLU:HB3	0.549
3	A:3:LEU:HD21	B:2:PRO:HG2	0.544
3	A:32:HIS:O	A:35:LEU:HG	0.535
3	B:41:SER:O	B:45:LYS:HG3	0.533

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:69:MET:O	B:2:PRO:HG3	0.528
3	A:43:LEU:HA	A:46:VAL:CG1	0.523
3	A:6:THR:HG23	B:46:ILE:HB	0.514
3	A:51:ILE:HD12	A:68:ARG:HD3	0.506
3	B:3:LEU:O	B:7:VAL:HG23	0.506
3	B:54:GLU:O	B:58:ARG:HG3	0.485
3	A:39:LEU:HD23	A:56:LEU:HD21	0.471
3	B:8:LEU:HG	B:12:LYS:HE3	0.468
3	A:11:ALA:O	A:15:LEU:HB2	0.464
3	B:22:THR:HA	B:62:VAL:HG22	0.452
3	B:1:ASN:O	B:4:GLU:HG2	0.450
3	A:49:VAL:HB	A:69:MET:HE3	0.445
3	A:5:THR:HG21	B:48:GLY:CA	0.439
3	B:59:HIS:ND1	B:64:GLN:HB3	0.437
3	A:4:ARG:HB2	A:4:ARG:NH1	0.434
3	B:9:GLN:CA	B:12:LYS:HD2	0.424
3	A:5:THR:HG21	B:48:GLY:HA3	0.420
3	B:65:LEU:O	B:69:VAL:HG23	0.419
3	A:20:LEU:HA	A:20:LEU:HD22	0.412
3	A:46:VAL:HG23	B:6:VAL:HB	0.409
3	A:61:THR:H	A:64:ASP:HB3	0.406
4	B:1:ASN:HB2	B:4:GLU:HB2	0.921
4	A:6:THR:HG23	B:46:ILE:HB	0.874

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	B:3:LEU:HD23	B:66:ALA:HA	0.758
4	A:6:THR:HG21	B:6:VAL:HG21	0.748
4	B:12:LYS:HZ2	B:18:ASP:HA	0.634
4	B:4:GLU:HG2	B:22:THR:HG21	0.611
4	B:3:LEU:O	B:7:VAL:HG23	0.595
4	A:43:LEU:HA	A:46:VAL:HG12	0.587
4	A:53:GLY:HA2	A:56:LEU:HB3	0.558
4	B:3:LEU:HB3	B:66:ALA:HB1	0.554
4	A:39:LEU:HD23	A:56:LEU:HD21	0.543
4	B:12:LYS:NZ	B:18:ASP:HA	0.542
4	A:3:LEU:HD21	B:3:LEU:HA	0.512
4	A:61:THR:H	A:64:ASP:HB3	0.506
4	A:32:HIS:O	A:35:LEU:HG	0.504
4	B:63:GLU:OE2	B:64:GLN:HG2	0.504
4	A:51:ILE:HD12	A:68:ARG:HD3	0.487
4	B:40:ALA:O	B:44:GLN:HG3	0.480
4	A:10:LEU:HD11	A:43:LEU:HD21	0.476
4	B:7:VAL:CG1	B:62:VAL:HB	0.472
4	A:6:THR:CG2	B:6:VAL:HG21	0.471
4	B:32:ASN:HB3	B:35:HIS:HB2	0.470
4	A:11:ALA:O	A:15:LEU:HB2	0.459
4	A:39:LEU:O	A:43:LEU:HG	0.458
4	B:8:LEU:HD13	B:22:THR:HG23	0.448

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:8:LEU:HD11	A:20:LEU:O	0.443
4	A:5:THR:HG21	B:48:GLY:CA	0.439
4	A:3:LEU:HD22	A:47:PHE:CE2	0.429
4	A:5:THR:HG21	B:48:GLY:HA2	0.428
4	B:12:LYS:O	B:16:GLY:HA2	0.428
4	B:39:LEU:O	B:43:LEU:HG	0.428
4	A:44:THR:HG22	A:50:GLU:HG2	0.427
4	B:22:THR:O	B:62:VAL:HG22	0.424
4	A:43:LEU:HA	A:46:VAL:CG1	0.422
4	A:3:LEU:HA	A:6:THR:OG1	0.417
4	B:54:GLU:O	B:58:ARG:HG3	0.410
4	A:3:LEU:O	A:7:VAL:HG23	0.409
4	A:26:LEU:O	A:30:CYS:HB2	0.408
4	A:3:LEU:HD23	B:3:LEU:HD12	0.406
5	B:1:ASN:HB2	B:4:GLU:HB2	0.792
5	A:3:LEU:HD21	B:3:LEU:HA	0.666
5	A:43:LEU:HA	A:46:VAL:HG12	0.659
5	A:6:THR:HG23	B:46:ILE:HB	0.652
5	B:44:GLN:HG2	B:51:VAL:H	0.634
5	A:1:SER:HB3	A:73:ARG:HH22	0.632
5	A:6:THR:HG21	B:6:VAL:HG21	0.597
5	B:12:LYS:HZ2	B:18:ASP:HA	0.573
5	A:32:HIS:O	A:35:LEU:HG	0.557

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:51:ILE:HD12	A:68:ARG:HD3	0.529
5	B:54:GLU:O	B:58:ARG:HG3	0.523
5	A:40:ALA:HA	A:43:LEU:HD12	0.522
5	A:6:THR:CG2	B:6:VAL:HG21	0.515
5	B:12:LYS:NZ	B:18:ASP:HA	0.512
5	A:39:LEU:O	A:43:LEU:HG	0.511
5	A:1:SER:HB3	A:73:ARG:NH2	0.510
5	B:32:ASN:HB3	B:35:HIS:HB2	0.498
5	B:27:LEU:H	B:27:LEU:HD12	0.489
5	A:61:THR:H	A:64:ASP:HB3	0.462
5	B:12:LYS:O	B:16:GLY:HA2	0.458
5	A:72:ARG:HB3	B:2:PRO:HA	0.456
5	B:22:THR:O	B:62:VAL:HG22	0.455
5	A:46:VAL:HA	B:9:GLN:HG3	0.444
5	B:39:LEU:O	B:43:LEU:HG	0.441
5	A:12:ARG:HB2	A:17:SER:O	0.436
5	B:3:LEU:O	B:7:VAL:HG23	0.434
5	B:40:ALA:O	B:44:GLN:HG3	0.433
5	A:5:THR:HG21	B:48:GLY:HA2	0.431
5	B:1:ASN:HB2	B:4:GLU:CB	0.430
5	B:63:GLU:OE2	B:64:GLN:HG2	0.424
5	A:8:LEU:HD13	A:62:VAL:HG21	0.411
5	A:3:LEU:CD2	B:3:LEU:HA	0.406

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:8:LEU:HD11	A:20:LEU:O	0.404
5	A:46:VAL:HG22	B:6:VAL:HG23	0.402
6	A:6:THR:HG23	B:46:ILE:HB	0.839
6	A:6:THR:HG21	B:6:VAL:HG21	0.826
6	B:1:ASN:HB2	B:4:GLU:HB2	0.807
6	A:43:LEU:HA	A:46:VAL:HG12	0.644
6	A:3:LEU:HD21	B:3:LEU:HA	0.635
6	B:12:LYS:HZ2	B:18:ASP:HA	0.584
6	B:39:LEU:O	B:43:LEU:HG	0.537
6	A:44:THR:HG22	A:50:GLU:HG2	0.536
6	B:12:LYS:NZ	B:18:ASP:HA	0.512
6	A:10:LEU:HD11	A:43:LEU:HD21	0.506
6	A:47:PHE:HB3	A:69:MET:HG2	0.506
6	A:51:ILE:HD12	A:68:ARG:HD3	0.506
6	A:32:HIS:O	A:35:LEU:HG	0.504
6	A:39:LEU:HD23	A:56:LEU:HD21	0.501
6	A:61:THR:H	A:64:ASP:HB3	0.499
6	B:3:LEU:O	B:7:VAL:HG23	0.493
6	B:8:LEU:HB3	B:62:VAL:HG21	0.487
6	A:43:LEU:HA	A:46:VAL:CG1	0.485
6	A:12:ARG:HB2	A:17:SER:O	0.475
6	B:53:THR:HA	B:56:VAL:HG22	0.474
6	A:47:PHE:C	B:5:THR:HG21	0.470

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:3:LEU:O	A:7:VAL:HG23	0.466
6	B:63:GLU:OE2	B:64:GLN:HG2	0.464
6	B:12:LYS:O	B:16:GLY:HA2	0.460
6	A:22:ALA:HA	A:62:VAL:HG22	0.451
6	A:53:GLY:HA2	A:56:LEU:HB3	0.451
6	B:40:ALA:O	B:44:GLN:HG3	0.443
6	A:47:PHE:C	A:49:VAL:H	0.438
6	B:32:ASN:HB3	B:35:HIS:HB2	0.436
6	B:43:LEU:HA	B:46:ILE:HG12	0.436
6	A:2:PRO:HG2	B:3:LEU:HD13	0.435
6	A:6:THR:HG23	B:46:ILE:CB	0.428
6	B:3:LEU:HD23	B:66:ALA:HA	0.426
6	A:26:LEU:O	A:30:CYS:HB2	0.425
6	A:3:LEU:HD23	B:3:LEU:HD12	0.423
6	B:47:PHE:HD1	B:51:VAL:HG21	0.414
6	A:3:LEU:HA	A:6:THR:OG1	0.413
6	B:41:SER:HA	B:44:GLN:OE1	0.410
6	A:46:VAL:HG22	B:6:VAL:HG23	0.407
6	A:72:ARG:HH21	B:1:ASN:N	0.406
6	B:24:ASP:O	B:61:THR:HA	0.404
6	A:2:PRO:HG3	B:70:GLU:HG2	0.402
6	A:6:THR:HB	A:47:PHE:HZ	0.402
7	B:8:LEU:HD12	B:12:LYS:HE2	0.673

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	B:9:GLN:HA	B:9:GLN:HE21	0.672
7	A:6:THR:HG23	B:46:ILE:HB	0.661
7	A:48:ALA:HB2	B:5:THR:HG21	0.631
7	B:3:LEU:HG	B:6:VAL:HG12	0.610
7	A:2:PRO:HG3	B:69:VAL:HG13	0.607
7	A:43:LEU:HA	A:46:VAL:HG12	0.607
7	A:3:LEU:HD21	B:3:LEU:HA	0.589
7	B:39:LEU:O	B:43:LEU:HG	0.546
7	A:6:THR:HG21	B:6:VAL:HG21	0.535
7	B:3:LEU:HD21	B:47:PHE:CZ	0.534
7	A:32:HIS:O	A:35:LEU:HG	0.529
7	A:10:LEU:HD11	A:43:LEU:HD21	0.503
7	A:39:LEU:O	A:43:LEU:HG	0.503
7	A:61:THR:H	A:64:ASP:HB3	0.486
7	A:1:SER:HB3	A:73:ARG:NH2	0.485
7	A:3:LEU:HD22	A:47:PHE:CE2	0.476
7	A:6:THR:HB	A:47:PHE:HZ	0.466
7	A:6:THR:HB	A:47:PHE:CZ	0.458
7	A:9:ASP:O	A:12:ARG:HG2	0.457
7	A:11:ALA:O	A:15:LEU:HB2	0.457
7	B:66:ALA:HA	B:69:VAL:HG12	0.451
7	A:49:VAL:HB	A:69:MET:HG3	0.448
7	B:54:GLU:OE1	B:58:ARG:HD3	0.447

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:3:LEU:O	A:7:VAL:HG23	0.444
7	A:51:ILE:HD12	A:68:ARG:HD3	0.441
7	A:26:LEU:O	A:30:CYS:HB2	0.438
7	B:1:ASN:HB2	B:4:GLU:HG3	0.422
7	A:3:LEU:HD23	B:3:LEU:HD12	0.419
7	A:2:PRO:HG2	B:3:LEU:HD13	0.417
7	A:1:SER:O	A:4:ARG:HB2	0.413
7	B:3:LEU:HG	B:6:VAL:CG1	0.413
7	A:46:VAL:HG22	B:6:VAL:HG23	0.409
7	A:5:THR:HG21	B:48:GLY:CA	0.402
7	B:3:LEU:HD22	B:69:VAL:CG1	0.402
7	B:59:HIS:ND1	B:64:GLN:HB3	0.402
8	A:6:THR:HG23	B:46:ILE:HB	0.923
8	A:6:THR:HB	A:47:PHE:HZ	0.839
8	B:1:ASN:HB2	B:4:GLU:HB2	0.777
8	B:8:LEU:HB3	B:62:VAL:HG21	0.667
8	B:44:GLN:HG2	B:51:VAL:H	0.621
8	A:44:THR:HG22	A:50:GLU:HG2	0.616
8	A:6:THR:HB	A:47:PHE:CZ	0.611
8	A:6:THR:HG21	B:6:VAL:HG21	0.607
8	A:39:LEU:HD23	A:56:LEU:HD21	0.588
8	B:12:LYS:HZ2	B:18:ASP:HA	0.567
8	A:61:THR:H	A:64:ASP:HB3	0.561

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:46:VAL:HG13	B:6:VAL:HG23	0.557
8	A:32:HIS:O	A:35:LEU:HG	0.552
8	B:1:ASN:HB2	B:4:GLU:CB	0.527
8	B:12:LYS:NZ	B:18:ASP:HA	0.513
8	A:51:ILE:HD12	A:68:ARG:HD3	0.505
8	B:54:GLU:O	B:58:ARG:HG3	0.500
8	B:7:VAL:HG21	B:66:ALA:HB2	0.487
8	B:32:ASN:HB3	B:35:HIS:HB2	0.485
8	B:27:LEU:H	B:27:LEU:HD12	0.474
8	A:6:THR:CG2	B:6:VAL:HG21	0.470
8	B:12:LYS:O	B:16:GLY:HA2	0.468
8	A:22:ALA:HA	A:62:VAL:HG22	0.456
8	B:39:LEU:O	B:43:LEU:HG	0.450
8	A:46:VAL:HA	B:9:GLN:HG3	0.440
8	A:43:LEU:HA	A:46:VAL:HB	0.429
8	A:12:ARG:HB2	A:17:SER:O	0.413
8	B:40:ALA:O	B:44:GLN:HG3	0.410
8	A:47:PHE:HA	B:5:THR:HG23	0.408
8	A:47:PHE:C	B:5:THR:HG21	0.406
8	B:3:LEU:O	B:6:VAL:HG12	0.401
9	A:6:THR:HG23	B:46:ILE:HB	0.731
9	B:1:ASN:HB2	B:4:GLU:HB2	0.682
9	B:12:LYS:HZ2	B:18:ASP:HA	0.661

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:6:THR:HG21	B:6:VAL:HG21	0.654
9	A:43:LEU:HA	A:46:VAL:HG12	0.580
9	A:6:THR:HB	A:47:PHE:HZ	0.572
9	B:44:GLN:HG2	B:51:VAL:H	0.568
9	A:10:LEU:HD11	A:43:LEU:HD21	0.560
9	B:12:LYS:NZ	B:18:ASP:HA	0.539
9	B:22:THR:O	B:62:VAL:HG22	0.526
9	B:39:LEU:O	B:43:LEU:HG	0.522
9	B:41:SER:HA	B:44:GLN:HG3	0.521
9	B:3:LEU:O	B:7:VAL:HG23	0.519
9	A:32:HIS:O	A:35:LEU:HG	0.515
9	A:51:ILE:HD12	A:68:ARG:HD3	0.512
9	A:6:THR:HB	A:47:PHE:CZ	0.506
9	A:3:LEU:HD22	A:47:PHE:HE2	0.498
9	A:40:ALA:HA	A:43:LEU:HD12	0.497
9	A:5:THR:HG21	B:48:GLY:HA2	0.493
9	A:3:LEU:HD21	B:3:LEU:HA	0.492
9	A:11:ALA:O	A:15:LEU:HB2	0.488
9	A:61:THR:H	A:64:ASP:HB3	0.486
9	B:43:LEU:HD23	B:46:ILE:HD11	0.485
9	B:3:LEU:HD23	B:66:ALA:HA	0.478
9	B:32:ASN:HB3	B:35:HIS:HB2	0.475
9	A:21:THR:HG22	A:22:ALA:H	0.450

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:3:LEU:HD22	A:47:PHE:CE2	0.440
9	B:12:LYS:O	B:16:GLY:HA2	0.439
9	B:7:VAL:CG1	B:62:VAL:HB	0.434
9	B:54:GLU:O	B:58:ARG:HG3	0.432
9	A:53:GLY:HA2	A:56:LEU:HB3	0.424
9	B:40:ALA:O	B:44:GLN:HG3	0.412
9	A:5:THR:HG21	B:48:GLY:CA	0.408
9	B:56:VAL:HG12	B:65:LEU:HD21	0.407
9	B:27:LEU:H	B:27:LEU:HD12	0.406
9	A:8:LEU:HD13	A:62:VAL:HG21	0.401
10	A:6:THR:HG23	B:46:ILE:HB	0.989
10	A:6:THR:HB	A:47:PHE:HZ	0.771
10	A:44:THR:HG22	A:50:GLU:HG2	0.746
10	A:46:VAL:HG22	B:6:VAL:HG23	0.683
10	B:1:ASN:HB2	B:4:GLU:HB2	0.681
10	A:43:LEU:HA	A:46:VAL:HG12	0.652
10	A:4:ARG:HE	A:63:ALA:HA	0.617
10	B:8:LEU:HB3	B:62:VAL:HG21	0.597
10	B:44:GLN:HG2	B:51:VAL:H	0.596
10	A:51:ILE:HD12	A:68:ARG:HD3	0.583
10	B:12:LYS:HZ2	B:18:ASP:HA	0.572
10	A:6:THR:HG21	B:6:VAL:HG21	0.570
10	B:1:ASN:HB2	B:4:GLU:CB	0.550

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:32:HIS:O	A:35:LEU:HG	0.549
10	B:32:ASN:HB3	B:35:HIS:HB2	0.530
10	B:12:LYS:NZ	B:18:ASP:HA	0.508
10	A:39:LEU:HD23	A:56:LEU:HD21	0.471
10	B:12:LYS:O	B:16:GLY:HA2	0.469
10	B:3:LEU:O	B:7:VAL:HG23	0.462
10	A:43:LEU:HA	A:46:VAL:CG1	0.459
10	B:39:LEU:O	B:43:LEU:HG	0.453
10	B:40:ALA:O	B:44:GLN:HG3	0.449
10	B:7:VAL:HG21	B:66:ALA:HB2	0.448
10	A:5:THR:HG21	B:48:GLY:HA2	0.445
10	A:8:LEU:HD11	A:20:LEU:O	0.445
10	A:47:PHE:C	B:5:THR:HG21	0.441
10	B:25:SER:HA	B:60:GLY:O	0.433
10	B:54:GLU:O	B:58:ARG:HG3	0.431
10	B:63:GLU:OE2	B:64:GLN:HG2	0.423
10	A:70:ASP:CG	A:73:ARG:HH12	0.421
10	A:6:THR:CG2	B:6:VAL:HG21	0.416
10	A:12:ARG:HB2	A:17:SER:O	0.416
10	A:61:THR:H	A:64:ASP:HB3	0.415
10	A:46:VAL:HA	B:9:GLN:HG3	0.412
10	B:3:LEU:O	B:6:VAL:HG12	0.405

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	141	131	9	1
2	141	131	8	2
3	141	131	9	1
4	141	132	8	1
5	141	129	11	1
6	141	132	8	1
7	141	131	9	1
8	141	132	9	0
9	141	134	7	0
10	141	132	7	2

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	117	81	18	18
2	117	84	16	17
3	117	83	16	18
4	117	84	10	23
5	117	87	14	16
6	117	87	12	18
7	117	82	13	22
8	117	89	11	17
9	117	84	18	15

Model ID	Analyzed	Favored	Allowed	Outliers
10	117	83	17	17

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	1	SER
1	А	4	ARG
1	A	5	THR
1	A	20	LEU
1	А	21	THR
1	А	28	ASP
1	А	37	ASP
1	А	52	THR
1	А	71	ASP
1	В	6	VAL
1	В	8	LEU
1	В	9	GLN
1	В	22	THR
1	В	23	THR
1	В	24	ASP
1	В	33	SER
1	В	52	SER
1	В	63	GLU
2	А	1	SER
2	А	4	ARG

Model ID	Chain	Residue ID	Residue type
2	А	5	THR
2	А	6	THR
2	А	20	LEU
2	A	28	ASP
2	A	71	ASP
2	В	6	VAL
2	В	8	LEU
2	В	22	THR
2	В	23	THR
2	В	24	ASP
2	В	33	SER
2	В	52	SER
2	В	53	THR
2	В	63	GLU
2	В	65	LEU
3	A	1	SER
3	A	5	THR
3	A	6	THR
3	A	20	LEU
3	A	21	THR
3	A	28	ASP
3	A	37	ASP
3	A	52	THR

Model ID	Chain	Residue ID	Residue type
3	A	62	VAL
3	А	71	ASP
3	В	8	LEU
3	В	13	ASP
3	В	21	THR
3	В	23	THR
3	В	33	SER
3	В	44	GLN
3	В	53	THR
3	В	62	VAL
4	А	1	SER
4	А	4	ARG
4	A	5	THR
4	A	6	THR
4	A	20	LEU
4	A	28	ASP
4	A	52	THR
4	А	62	VAL
4	A	71	ASP
4	В	5	THR
4	В	8	LEU
4	В	9	GLN
4	В	18	ASP

Model ID	Chain	Residue ID	Residue type
4	В	19	ASP
4	В	22	THR
4	В	23	THR
4	В	24	ASP
4	В	33	SER
4	В	41	SER
4	В	45	LYS
4	В	52	SER
4	В	53	THR
4	В	63	GLU
5	A	1	SER
5	A	4	ARG
5	A	5	THR
5	A	20	LEU
5	A	21	THR
5	A	28	ASP
5	A	52	THR
5	A	71	ASP
5	В	8	LEU
5	В	22	THR
5	В	23	THR
5	В	24	ASP
5	В	33	SER

Model ID	Chain	Residue ID	Residue type
5	В	52	SER
5	В	53	THR
5	В	63	GLU
6	A	1	SER
6	А	4	ARG
6	A	5	THR
6	A	6	THR
6	А	20	LEU
6	А	21	THR
6	A	28	ASP
6	A	52	THR
6	A	62	VAL
6	В	8	LEU
6	В	9	GLN
6	В	22	THR
6	В	23	THR
6	В	24	ASP
6	В	33	SER
6	В	52	SER
6	В	53	THR
6	В	63	GLU
7	A	1	SER
7	A	4	ARG

Model ID	Chain	Residue ID	Residue type
7	А	5	THR
7	A	6	THR
7	A	20	LEU
7	А	21	THR
7	А	28	ASP
7	А	52	THR
7	А	71	ASP
7	В	3	LEU
7	В	5	THR
7	В	6	VAL
7	В	8	LEU
7	В	9	GLN
7	В	21	THR
7	В	22	THR
7	В	23	THR
7	В	25	SER
7	В	29	HIS
7	В	33	SER
7	В	53	THR
7	В	68	PHE
8	А	5	THR
8	А	6	THR
8	А	20	LEU

Model ID	Chain	Residue ID	Residue type
8	A	21	THR
8	А	28	ASP
8	A	52	THR
8	А	62	VAL
8	В	9	GLN
8	В	18	ASP
8	В	19	ASP
8	В	22	THR
8	В	23	THR
8	В	24	ASP
8	В	33	SER
8	В	52	SER
8	В	53	THR
8	В	63	GLU
9	А	4	ARG
9	A	5	THR
9	A	6	THR
9	А	20	LEU
9	A	28	ASP
9	A	70	ASP
9	A	71	ASP
9	В	8	LEU
9	В	22	THR

Model ID	Chain	Residue ID	Residue type
9	В	23	THR
9	В	24	ASP
9	В	33	SER
9	В	52	SER
9	В	53	THR
9	В	63	GLU
10	А	5	THR
10	А	6	THR
10	А	20	LEU
10	А	28	ASP
10	А	46	VAL
10	А	52	THR
10	А	62	VAL
10	А	71	ASP
10	В	8	LEU
10	В	9	GLN
10	В	22	THR
10	В	23	THR
10	В	24	ASP
10	В	33	SER
10	В	52	SER
10	В	53	THR
10	В	63	GLU

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

<u>NMR</u>

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.