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	9A82
PDB-Dev ID	PDBDEV_00000367
Structure Title	Tomaymycin NRPS system: complex of the substrate-loaded peptidyl-carrier-protein domain from the A module (APCP-load) with the adaptor (BN91) and condensation (BC) domains of the B 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

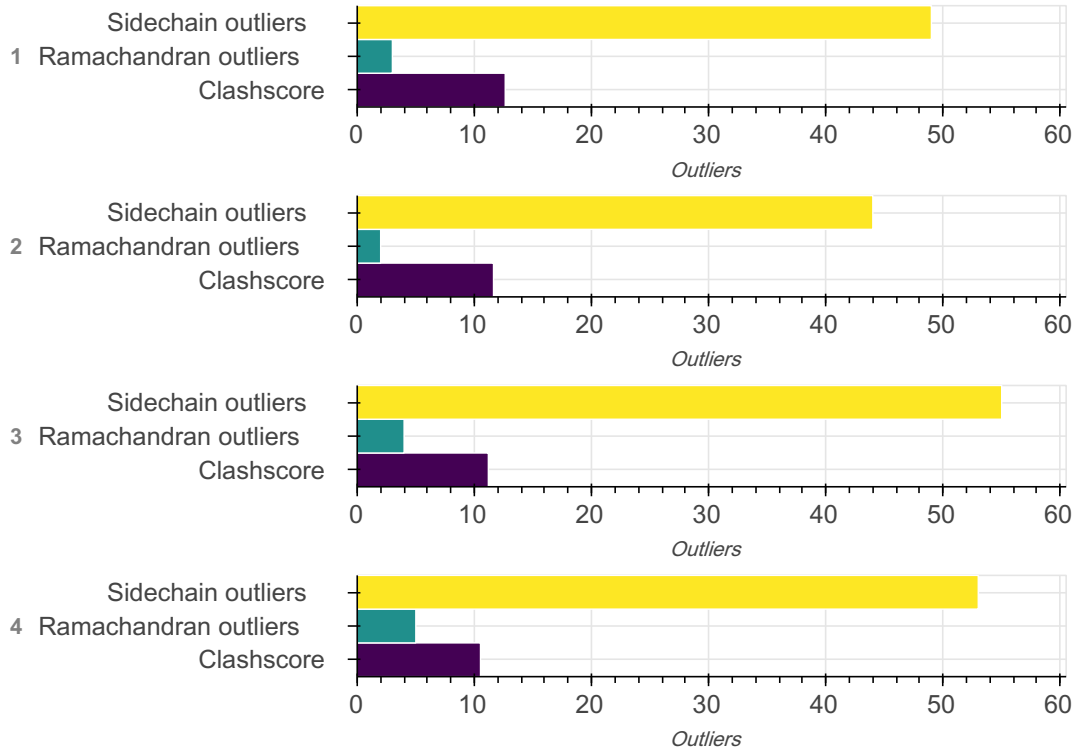
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

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 4 unique models, with 3 subunits in each model. A total of 7 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 3 flexible or non-rigid units.

Entry composition

There are 4 unique types of models in this entry.These models are titled None, None, None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module	A	A	76
1	2	2	Substrate-loaded peptidyl-carrier-protein (APCP) domain of the Tomaymycin A module	B	B	75

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	3	1	Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module	A	A	432
2	1	1	Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module	A	A	76
2	2	2	Substrate-loaded peptidyl-carrier-protein (APCP) domain of the Tomaymycin A module	B	B	75
2	3	1	Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module	A	A	432
3	1	1	Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module	A	A	76
3	2	2	Substrate-loaded peptidyl-carrier-protein (APCP) domain of the Tomaymycin A module	B	B	75
3	3	1	Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module	A	A	432
4	1	1	Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module	A	A	76
4	2	2	Substrate-loaded peptidyl-carrier-protein (APCP) domain of the Tomaymycin A module	B	B	75
4	3	1	Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module	A	A	432

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	NMR data	Not available	Not available
2	Other	Not available	Not available
3	NMR data	Not available	Not available

ID	Dataset type	Database name	Data access code
4	Other	Not available	Not available
5	Experimental model	PDB	8QSX
6	Experimental model	PDB	8QNF
7	Experimental model	PDB	8QRX

Representation

This entry has only one representation and includes 0 rigid bodies and 3 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-76, 77-508
B	-	1-75

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	Data-driven docking using PRE-derived distance restraints within HADDOCK.	None	Step 1: docking of BC domain and APCP to form a binary BC-APCP complex (representing the starting models for step 2).	None	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
2	1	Data-driven docking using PRE-derived distance restraints within HADDOCK.	None	Step 2: docking of BN91 domain to binary BC-APCP complex generated in step 1.	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/

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 4062 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--H2	1.04	0.96	2
N--H3	1.05	0.96	1
N--H3	1.06	0.96	3
N--H	0.97	0.86	6
NE2--HE22	0.97	0.86	3

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N--H	0.98	0.86	1991
ND2--HD22	0.98	0.86	38
NE2--HE22	0.98	0.86	65
NE--HE	0.98	0.86	134
NE2--HE21	0.98	0.86	52
ND1--HD1	0.98	0.86	36
NE2--HE2	0.98	0.86	34
NE1--HE1	0.98	0.86	16
ND2--HD21	0.98	0.86	40
OH--HH	0.96	0.84	38
OG1--HG1	0.96	0.84	78
OG--HG	0.96	0.84	58
SG--HG	1.32	1.20	5
NE2--HE2	0.99	0.86	14
N--H	0.99	0.86	203
ND2--HD22	0.99	0.86	2
OG--HG	0.97	0.84	37
ND1--HD1	0.99	0.86	27
OH--HH	0.97	0.84	10
NE--HE	0.99	0.86	56
OG1--HG1	0.97	0.84	50
SG--HG	1.33	1.20	7
NE2--HE21	0.99	0.86	16

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE22	0.99	0.86	4
NH2--HH21	0.99	0.86	4
NH2--HH22	0.99	0.86	9
NH1--HH11	0.99	0.86	2
NH1--HH12	0.99	0.86	2
NE--HE	1.00	0.86	30
NH2--HH21	1.00	0.86	132
NH1--HH12	1.00	0.86	149
NH1--HH11	1.00	0.86	135
NH2--HH22	1.00	0.86	117
OG1--HG1	0.98	0.84	12
NE2--HE2	1.00	0.86	8
OG--HG	0.98	0.84	9
ND1--HD1	1.00	0.86	9
NE2--HE21	1.00	0.86	4
NZ--HZ1	1.03	0.89	1
NZ--HZ2	1.03	0.89	5
NZ--HZ3	1.03	0.89	2
NH1--HH11	1.01	0.86	41
NH2--HH22	1.01	0.86	57
NZ--HZ1	1.04	0.89	20
NH1--HH12	1.01	0.86	46
NH2--HH21	1.01	0.86	50

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ2	1.04	0.89	13
NZ--HZ3	1.04	0.89	16
NH2--HH22	1.02	0.86	37
NZ--HZ2	1.05	0.89	10
NH1--HH11	1.02	0.86	42
NH2--HH21	1.02	0.86	34
NZ--HZ1	1.05	0.89	7
NH1--HH12	1.02	0.86	23
NZ--HZ3	1.05	0.89	10

Standard geometry: angle outliers

There are 6 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
CA-N-CD	112.00	103.47	1
CA-N-CD	112.00	103.69	1
CA-N-CD	112.00	103.73	1
CA-N-CD	112.00	104.28	1
N-CA-CB	103.00	107.95	1
N-CA-CB	103.00	107.42	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	12.63	114
2	11.63	105

Model ID	Clash score	Number of clashes
3	11.19	101
4	10.52	95

All 415 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:376:THR:HA	A:501:PRO:HA	0.881
1	B:32:WP9:N13	B:32:WP9:S44	0.817
1	A:305:ALA:HB1	A:464:LEU:HB3	0.783
1	A:301:PRO:HD3	A:488:ARG:HD3	0.725
1	A:97:PRO:HB3	A:450:LYS:HB2	0.718
1	A:493:GLN:HB3	A:505:LEU:HD22	0.705
1	A:318:THR:HG22	B:56:PHE:HB3	0.685
1	A:106:VAL:HG11	A:218:LEU:HD11	0.684
1	A:7:THR:HB	A:48:PHE:HZ	0.680
1	B:11:LYS:HG2	B:17:ASP:HA	0.678
1	A:497:ARG:NH2	A:504:GLU:HB3	0.668
1	A:377:VAL:HB	A:498:PRO:HA	0.667
1	A:44:LEU:HA	A:47:VAL:HG12	0.657
1	A:210:ASP:HA	B:32:WP9:S44	0.651
1	A:155:PHE:HA	A:188:VAL:O	0.641
1	A:311:LEU:HD22	A:495:ALA:HA	0.638
1	A:7:THR:HB	A:48:PHE:CZ	0.622
1	A:101:ASN:HA	B:32:WP9:O11	0.614
1	A:267:ALA:HA	A:406:LEU:HD21	0.613

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:33:HIS:CE1	A:35:ALA:HB3	0.612
1	A:477:GLU:HB3	A:478:PRO:HD3	0.611
1	A:26:PRO:HB2	A:29:ASP:HB3	0.597
1	A:129:GLU:HA	A:132:ARG:NH1	0.595
1	A:16:LEU:HD12	A:31:CYS:HB3	0.594
1	A:22:THR:H	A:25:GLU:HG3	0.587
1	A:219:ARG:HD2	A:356:GLU:OE1	0.587
1	B:8:GLN:HA	B:11:LYS:HD2	0.583
1	A:497:ARG:HH22	A:504:GLU:HB3	0.579
1	A:269:ARG:HH22	A:390:GLU:HG3	0.577
1	A:10:ASP:O	A:13:ARG:HG2	0.570
1	A:270:LEU:HB3	A:274:LEU:HD11	0.569
1	A:84:GLN:HG2	A:207:ILE:HG12	0.566
1	A:385:ARG:HH21	A:386:GLU:CD	0.565
1	A:354:THR:HA	A:357:LEU:HD12	0.563
1	A:103:PRO:HG2	A:174:ALA:HA	0.562
1	A:321:MET:HG2	A:385:ARG:HA	0.560
1	A:107:ARG:HD2	A:442:GLU:OE2	0.559
1	A:66:VAL:HG12	A:70:MET:HE3	0.555
1	A:36:LEU:HA	A:39:ASP:OD2	0.547
1	A:22:THR:H	A:25:GLU:CG	0.541
1	A:50:VAL:HG11	A:70:MET:HG2	0.532
1	A:347:SER:HB2	B:32:WP9:C33	0.532

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:23:ALA:HA	A:63:VAL:HG22	0.530
1	A:407:GLN:N	A:408:PRO:HD3	0.530
1	A:104:PHE:HB3	A:443:ARG:HD3	0.529
1	A:40:LEU:O	A:44:LEU:HG	0.524
1	A:224:ALA:HA	A:234:VAL:HG21	0.520
1	A:254:MET:HA	A:254:MET:HE2	0.520
1	A:4:LEU:O	A:8:VAL:HG23	0.514
1	A:117:LEU:O	A:121:VAL:HG23	0.512
1	A:255:ASN:HB2	A:256:PRO:HD2	0.509
1	B:38:LEU:O	B:42:LEU:HG	0.507
1	A:362:VAL:HG21	B:32:WP9:C39	0.503
1	A:351:ASP:OD2	A:352:PRO:HD2	0.499
1	A:454:SER:HB2	A:469:GLU:HB2	0.493
1	A:40:LEU:HD23	A:57:LEU:HD21	0.492
1	A:94:LEU:HB3	A:95:PRO:HD2	0.489
1	B:6:VAL:HG22	B:46:PHE:CZ	0.483
1	B:53:GLU:O	B:57:ARG:HG2	0.482
1	A:443:ARG:HH12	B:32:WP9:C14	0.481
1	A:80:ALA:HA	A:144:GLN:NE2	0.480
1	A:262:SER:HA	A:394:HIS:ND1	0.480
1	A:4:LEU:HD12	A:48:PHE:CD2	0.479
1	A:26:PRO:HD2	A:30:ARG:CG	0.479
1	B:58:HIS:ND1	B:63:GLN:HB3	0.477

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:29:ASP:OD1	A:30:ARG:HG2	0.475
1	A:160:TYR:O	A:193:GLY:HA2	0.474
1	A:47:VAL:HG13	A:48:PHE:CD1	0.473
1	A:218:LEU:HD13	A:221:LEU:HD23	0.472
1	A:335:THR:HB	A:337:GLN:HG3	0.470
1	A:33:HIS:O	A:36:LEU:HG	0.469
1	A:165:GLU:O	A:169:LEU:HG	0.468
1	A:401:LYS:HZ2	A:404:GLU:CD	0.464
1	A:309:GLU:HG2	A:319:LEU:HD13	0.463
1	A:127:ARG:HD2	A:234:VAL:HG12	0.461
1	A:16:LEU:HD13	A:36:LEU:HD11	0.460
1	A:3:PRO:HG2	A:4:LEU:HD22	0.459
1	A:389:SER:O	A:393:ARG:HG3	0.459
1	A:352:PRO:O	A:355:HIS:HB2	0.457
1	A:470:TYR:CG	A:480:VAL:HG21	0.457
1	A:23:ALA:HA	A:63:VAL:CG2	0.453
1	A:132:ARG:HD2	A:149:ASP:O	0.451
1	A:321:MET:SD	A:385:ARG:HG3	0.449
1	A:122:ARG:HB3	A:150:ASP:OD2	0.448
1	A:104:PHE:HB2	A:441:ILE:HG22	0.446
1	A:372:ASP:OD2	A:375:MET:HE3	0.439
1	B:2:LEU:O	B:5:VAL:HG12	0.437
1	A:61:ALA:HB1	A:66:VAL:HG22	0.436

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:291:HIS:O	A:448:GLY:HA2	0.436
1	A:26:PRO:HD2	A:30:ARG:HG3	0.435
1	A:281:THR:HG21	A:474:LEU:HB3	0.435
1	A:316:GLY:C	B:57:ARG:HB2	0.433
1	A:243:TYR:CE1	A:359:GLY:HA3	0.431
1	A:189:THR:HB	A:201:ILE:HB	0.429
1	A:481:ARG:HD3	A:485:ASP:OD1	0.429
1	A:286:PRO:HA	A:287:PRO:HD3	0.426
1	A:4:LEU:HG	A:70:MET:HB3	0.424
1	A:380:VAL:HG11	A:502:LEU:HD11	0.424
1	A:11:LEU:HD21	A:48:PHE:HE1	0.419
1	B:46:PHE:CD1	B:68:VAL:HG21	0.419
1	A:218:LEU:HB2	A:221:LEU:HB3	0.416
1	A:388:VAL:O	A:392:LEU:HG	0.414
1	A:500:ALA:HA	A:501:PRO:HD3	0.413
1	A:13:ARG:HH11	A:352:PRO:HD3	0.413
1	A:159:ARG:HA	A:192:LEU:O	0.412
1	A:279:LEU:HA	A:280:PRO:HD3	0.410
1	A:99:ALA:H	A:469:GLU:CD	0.409
1	A:278:ASP:O	A:335:THR:HG22	0.407
1	A:62:THR:O	A:66:VAL:HG23	0.405
1	A:455:LEU:HD11	A:468:ILE:HG12	0.405
1	A:23:ALA:HB3	A:239:LEU:HB3	0.404

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:485:ASP:CG	A:488:ARG:HH12	0.404
1	A:4:LEU:HD12	A:48:PHE:HD2	0.403
1	A:13:ARG:NH1	A:352:PRO:HD3	0.401
2	A:376:THR:HA	A:501:PRO:HA	0.856
2	B:32:WP9:N13	B:32:WP9:S44	0.822
2	A:305:ALA:HB1	A:464:LEU:HB3	0.787
2	A:16:LEU:HD12	A:31:CYS:HB3	0.710
2	A:318:THR:HG22	B:56:PHE:HB3	0.706
2	A:33:HIS:O	A:36:LEU:HG	0.699
2	A:106:VAL:HG11	A:218:LEU:HD11	0.684
2	B:11:LYS:HG2	B:17:ASP:HA	0.679
2	A:103:PRO:HG2	A:174:ALA:HA	0.669
2	A:493:GLN:HB3	A:505:LEU:HD22	0.657
2	A:210:ASP:HA	B:32:WP9:S44	0.654
2	A:301:PRO:HD3	A:488:ARG:HD3	0.648
2	A:377:VAL:HB	A:498:PRO:HA	0.639
2	A:155:PHE:HA	A:188:VAL:O	0.637
2	A:44:LEU:HA	A:47:VAL:HG12	0.636
2	A:454:SER:HB2	A:469:GLU:HB2	0.631
2	A:61:ALA:HB1	A:66:VAL:HG22	0.615
2	A:267:ALA:HA	A:406:LEU:HD21	0.608
2	A:101:ASN:HA	B:32:WP9:O11	0.590
2	A:321:MET:HG2	A:385:ARG:HA	0.588

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:66:VAL:HG12	A:70:MET:HE3	0.584
2	A:40:LEU:O	A:44:LEU:HG	0.579
2	A:5:ARG:HD3	A:67:ALA:HB3	0.578
2	A:26:PRO:HB2	A:29:ASP:HB3	0.578
2	A:477:GLU:HB3	A:478:PRO:HD3	0.578
2	A:497:ARG:NH2	A:504:GLU:HB3	0.574
2	A:22:THR:H	A:25:GLU:HG3	0.568
2	A:311:LEU:HD22	A:495:ALA:HA	0.568
2	A:84:GLN:HG2	A:207:ILE:HG12	0.566
2	A:97:PRO:HB3	A:450:LYS:HB2	0.557
2	A:10:ASP:O	A:13:ARG:HG2	0.555
2	A:347:SER:HB2	B:32:WP9:C33	0.547
2	A:107:ARG:HD2	A:442:GLU:OE2	0.539
2	A:269:ARG:HH22	A:390:GLU:HG3	0.538
2	A:270:LEU:HB3	A:274:LEU:HD11	0.537
2	A:407:GLN:N	A:408:PRO:HD3	0.533
2	A:362:VAL:HG21	B:32:WP9:C39	0.530
2	A:218:LEU:HD13	A:221:LEU:HD23	0.526
2	A:497:ARG:HH22	A:504:GLU:HB3	0.526
2	A:254:MET:HA	A:254:MET:HE2	0.525
2	B:38:LEU:O	B:42:LEU:HG	0.514
2	A:321:MET:SD	A:385:ARG:HG3	0.512
2	A:4:LEU:O	A:8:VAL:HG23	0.511

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:262:SER:HA	A:394:HIS:ND1	0.510
2	B:53:GLU:O	B:57:ARG:HG2	0.500
2	A:117:LEU:O	A:121:VAL:HG23	0.499
2	A:219:ARG:HD2	A:356:GLU:OE1	0.499
2	A:36:LEU:HA	A:39:ASP:OD2	0.495
2	A:62:THR:O	A:66:VAL:HG23	0.494
2	A:255:ASN:HB2	A:256:PRO:HD2	0.494
2	B:6:VAL:HG22	B:46:PHE:CZ	0.489
2	A:165:GLU:O	A:169:LEU:HG	0.488
2	B:8:GLN:HA	B:11:LYS:HD2	0.488
2	B:58:HIS:ND1	B:63:GLN:HB3	0.486
2	A:40:LEU:HD23	A:57:LEU:HD21	0.485
2	A:354:THR:HA	A:357:LEU:HD12	0.481
2	A:104:PHE:HB3	A:443:ARG:HD3	0.477
2	A:335:THR:HB	A:337:GLN:HG3	0.474
2	A:316:GLY:C	B:57:ARG:HB2	0.470
2	A:47:VAL:HG13	A:48:PHE:CD1	0.469
2	A:291:HIS:O	A:448:GLY:HA2	0.468
2	A:389:SER:O	A:393:ARG:HG3	0.466
2	A:189:THR:HB	A:201:ILE:HB	0.464
2	A:224:ALA:HA	A:234:VAL:HG21	0.461
2	B:46:PHE:CD1	B:68:VAL:HG21	0.459
2	A:309:GLU:HG2	A:319:LEU:HD13	0.458

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:127:ARG:HD2	A:234:VAL:HG12	0.457
2	A:94:LEU:HB3	A:95:PRO:HD2	0.455
2	A:372:ASP:OD2	A:375:MET:HE3	0.453
2	A:80:ALA:HA	A:144:GLN:NE2	0.451
2	A:7:THR:HB	A:48:PHE:CZ	0.448
2	A:481:ARG:HD3	A:485:ASP:OD1	0.448
2	A:132:ARG:HD2	A:149:ASP:O	0.447
2	A:4:LEU:HD12	A:48:PHE:HD2	0.445
2	A:25:GLU:HA	A:26:PRO:HD3	0.445
2	A:380:VAL:HG11	A:502:LEU:HD11	0.445
2	A:7:THR:HB	A:48:PHE:HZ	0.443
2	A:470:TYR:CG	A:480:VAL:HG21	0.439
2	A:104:PHE:HB2	A:441:ILE:HG22	0.437
2	A:218:LEU:HB2	A:221:LEU:HB3	0.434
2	A:28:ALA:HB2	A:58:ALA:HB1	0.430
2	A:122:ARG:HB3	A:150:ASP:OD2	0.430
2	A:206:HIS:HA	B:32:WP9:N13	0.430
2	A:388:VAL:O	A:392:LEU:HG	0.429
2	A:160:TYR:O	A:193:GLY:HA2	0.428
2	A:339:ARG:HG2	A:370:GLU:HG2	0.428
2	A:443:ARG:HH12	B:32:WP9:C14	0.428
2	A:129:GLU:HA	A:132:ARG:NH1	0.426
2	A:7:THR:O	A:11:LEU:HG	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:3:PRO:HG2	A:4:LEU:HD22	0.422
2	A:286:PRO:HA	A:287:PRO:HD3	0.419
2	A:278:ASP:O	A:335:THR:HG22	0.418
2	A:295:THR:HG22	A:469:GLU:HG2	0.417
2	A:159:ARG:HA	A:192:LEU:O	0.415
2	A:500:ALA:HA	A:501:PRO:HD3	0.413
2	A:237:ASP:HB3	A:240:ARG:HB3	0.412
2	A:279:LEU:HA	A:280:PRO:HD3	0.411
2	A:281:THR:HG21	A:474:LEU:HB3	0.410
2	A:4:LEU:HD12	A:48:PHE:CD2	0.408
2	A:9:LEU:HD13	A:63:VAL:HG21	0.405
2	A:152:ALA:O	A:184:PRO:HB3	0.405
2	A:162:ASP:OD2	A:164:LYS:HB3	0.405
2	A:19:ALA:HA	B:37:GLN:HG3	0.404
2	A:476:ASP:O	A:480:VAL:HG23	0.403
2	A:212:ALA:HB3	A:349:ARG:NE	0.402
3	A:376:THR:HA	A:501:PRO:HA	0.872
3	A:311:LEU:HD22	A:495:ALA:HA	0.767
3	A:7:THR:HB	A:48:PHE:HZ	0.753
3	A:377:VAL:HB	A:498:PRO:HA	0.752
3	A:26:PRO:HD2	A:30:ARG:HG3	0.721
3	A:493:GLN:HB3	A:505:LEU:HD22	0.718
3	A:26:PRO:HB2	A:29:ASP:HB3	0.710

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:497:ARG:NH2	A:504:GLU:HB3	0.705
3	A:301:PRO:HD3	A:488:ARG:HD3	0.676
3	A:267:ALA:HA	A:406:LEU:HD21	0.664
3	B:11:LYS:HG2	B:17:ASP:HA	0.658
3	A:44:LEU:HA	A:47:VAL:HG12	0.657
3	A:7:THR:HB	A:48:PHE:CZ	0.655
3	B:55:VAL:HA	B:64:LEU:HD21	0.650
3	A:477:GLU:HB3	A:478:PRO:HD3	0.643
3	A:321:MET:HG2	A:385:ARG:HA	0.638
3	A:106:VAL:HG11	A:218:LEU:HD11	0.637
3	A:40:LEU:HD23	A:57:LEU:HD21	0.630
3	A:22:THR:H	A:25:GLU:HG3	0.626
3	A:305:ALA:HB1	A:464:LEU:HB3	0.612
3	A:97:PRO:HB3	A:450:LYS:HB2	0.608
3	A:321:MET:HE1	B:53:GLU:HG3	0.606
3	A:129:GLU:HA	A:132:ARG:NH1	0.594
3	A:33:HIS:O	A:36:LEU:HG	0.590
3	A:155:PHE:HA	A:188:VAL:O	0.587
3	A:10:ASP:O	A:13:ARG:HG2	0.579
3	A:454:SER:HB2	A:469:GLU:HB2	0.574
3	A:84:GLN:HG2	A:207:ILE:HG12	0.573
3	A:32:GLU:CD	A:32:GLU:H	0.572
3	A:321:MET:SD	A:385:ARG:HG3	0.572

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:16:LEU:HD12	A:31:CYS:HB3	0.570
3	A:269:ARG:HH22	A:390:GLU:HG3	0.569
3	B:53:GLU:OE1	B:57:ARG:HD3	0.568
3	A:462:GLU:CD	A:463:GLY:H	0.564
3	A:497:ARG:HH22	A:504:GLU:HB3	0.563
3	A:40:LEU:O	A:44:LEU:HG	0.560
3	A:224:ALA:HA	A:234:VAL:HG21	0.560
3	A:160:TYR:O	A:193:GLY:HA2	0.545
3	A:36:LEU:HA	A:39:ASP:OD2	0.543
3	A:22:THR:N	A:25:GLU:HG3	0.540
3	A:407:GLN:N	A:408:PRO:HD3	0.535
3	A:254:MET:HA	A:254:MET:HE2	0.534
3	B:38:LEU:O	B:42:LEU:HG	0.534
3	A:117:LEU:O	A:121:VAL:HG23	0.529
3	A:4:LEU:O	A:8:VAL:HG23	0.521
3	A:21:LEU:HD13	A:25:GLU:HB2	0.517
3	A:26:PRO:HD2	A:30:ARG:CG	0.517
3	A:189:THR:HB	A:201:ILE:HB	0.514
3	A:11:LEU:HD21	A:48:PHE:HE1	0.512
3	A:255:ASN:HB2	A:256:PRO:HD2	0.503
3	A:218:LEU:HD13	A:221:LEU:HD23	0.500
3	B:8:GLN:HA	B:11:LYS:HD2	0.500
3	A:262:SER:HA	A:394:HIS:ND1	0.495

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:104:PHE:HB2	A:441:ILE:HG22	0.494
3	A:339:ARG:HG2	A:370:GLU:HG2	0.492
3	A:132:ARG:HD2	A:149:ASP:O	0.484
3	A:362:VAL:HG21	B:32:WP9:N41	0.482
3	A:122:ARG:HB3	A:150:ASP:OD2	0.479
3	A:127:ARG:HD2	A:234:VAL:HG12	0.478
3	A:61:ALA:HB1	A:66:VAL:HG22	0.477
3	A:335:THR:HB	A:337:GLN:HG3	0.474
3	A:21:LEU:HA	A:25:GLU:HG3	0.468
3	A:165:GLU:O	A:169:LEU:HG	0.467
3	A:28:ALA:HB2	A:58:ALA:HB1	0.455
3	A:470:TYR:CG	A:480:VAL:HG21	0.454
3	A:389:SER:O	A:393:ARG:HG3	0.452
3	A:458:GLU:HB2	A:465:HIS:CE1	0.451
3	B:2:LEU:O	B:5:VAL:HG12	0.450
3	A:66:VAL:HG12	A:70:MET:HE3	0.448
3	A:388:VAL:O	A:392:LEU:HG	0.435
3	A:425:THR:HG22	A:429:ALA:HB1	0.435
3	A:159:ARG:HA	A:192:LEU:O	0.434
3	A:218:LEU:HB2	A:221:LEU:HB3	0.434
3	A:503:HIS:HD2	A:504:GLU:HG3	0.433
3	A:372:ASP:OD2	A:375:MET:HE3	0.431
3	A:351:ASP:HB3	A:354:THR:OG1	0.430

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:354:THR:HA	A:357:LEU:HD12	0.429
3	A:500:ALA:HA	A:501:PRO:HD3	0.429
3	A:318:THR:HG22	B:56:PHE:HB3	0.428
3	A:107:ARG:HD2	A:442:GLU:OE2	0.426
3	B:54:ASP:HA	B:57:ARG:CZ	0.425
3	A:219:ARG:HD2	A:356:GLU:OE1	0.423
3	B:69:GLU:O	B:72:ARG:HG2	0.423
3	A:29:ASP:OD1	A:30:ARG:HG2	0.422
3	A:401:LYS:HZ2	A:404:GLU:CD	0.421
3	A:106:VAL:HG12	A:200:VAL:HB	0.420
3	B:6:VAL:HG22	B:46:PHE:CZ	0.420
3	A:80:ALA:HA	A:144:GLN:NE2	0.419
3	B:46:PHE:CD1	B:68:VAL:HG21	0.418
3	A:47:VAL:HG13	A:48:PHE:CD1	0.415
3	B:21:THR:HA	B:61:VAL:CG2	0.414
3	A:135:TYR:HB3	A:142:LEU:HD11	0.413
3	A:62:THR:O	A:66:VAL:HG23	0.411
3	A:100:TYR:CZ	A:423:VAL:HG21	0.409
3	A:320:PHE:O	A:324:VAL:HG23	0.408
3	A:485:ASP:CG	A:488:ARG:HH12	0.408
3	B:1:PRO:N	B:69:GLU:OE2	0.406
3	B:13:ILE:CD1	B:38:LEU:HA	0.405
3	A:152:ALA:O	A:184:PRO:HB3	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:325:ALA:O	A:329:VAL:HG23	0.402
3	A:279:LEU:HA	A:280:PRO:HD3	0.400
4	A:376:THR:HA	A:501:PRO:HA	0.837
4	A:26:PRO:HB2	A:29:ASP:HB3	0.767
4	A:22:THR:H	A:25:GLU:HG3	0.752
4	A:377:VAL:HB	A:498:PRO:HA	0.747
4	B:13:ILE:HG13	B:41:ARG:HH21	0.737
4	A:311:LEU:HD22	A:495:ALA:HA	0.733
4	A:7:THR:HB	A:48:PHE:HZ	0.688
4	A:497:ARG:NH2	A:504:GLU:HB3	0.684
4	A:7:THR:HB	A:48:PHE:CZ	0.666
4	A:493:GLN:HB3	A:505:LEU:HD22	0.665
4	A:106:VAL:HG11	A:218:LEU:HD11	0.659
4	A:321:MET:HG2	A:385:ARG:HA	0.655
4	A:305:ALA:HB1	A:464:LEU:HB3	0.652
4	A:44:LEU:HA	A:47:VAL:HG12	0.644
4	B:55:VAL:HA	B:64:LEU:HD21	0.639
4	A:267:ALA:HA	A:406:LEU:HD21	0.628
4	A:477:GLU:HB3	A:478:PRO:HD3	0.622
4	A:97:PRO:HB3	A:450:LYS:HB2	0.605
4	A:497:ARG:HH22	A:504:GLU:HB3	0.602
4	A:22:THR:N	A:25:GLU:HG3	0.599
4	A:33:HIS:O	A:36:LEU:HG	0.598

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:454:SER:HB2	A:469:GLU:HB2	0.591
4	A:155:PHE:HA	A:188:VAL:O	0.584
4	A:40:LEU:HD23	A:57:LEU:HD21	0.582
4	B:9:ALA:HB1	B:41:ARG:HD2	0.581
4	A:462:GLU:CD	A:463:GLY:H	0.577
4	A:40:LEU:O	A:44:LEU:HG	0.571
4	B:53:GLU:OE1	B:57:ARG:HD3	0.571
4	A:129:GLU:HA	A:132:ARG:NH1	0.567
4	A:36:LEU:HA	A:39:ASP:OD2	0.565
4	A:269:ARG:HH22	A:390:GLU:HG3	0.563
4	A:301:PRO:HD3	A:488:ARG:HD3	0.560
4	A:321:MET:SD	A:385:ARG:HG3	0.556
4	A:84:GLN:HG2	A:207:ILE:HG12	0.553
4	A:339:ARG:HG2	A:370:GLU:HG2	0.550
4	A:321:MET:HE1	B:53:GLU:HG3	0.544
4	A:407:GLN:N	A:408:PRO:HD3	0.535
4	A:254:MET:HA	A:254:MET:HE2	0.533
4	A:4:LEU:O	A:8:VAL:HG23	0.532
4	A:10:ASP:O	A:13:ARG:HG2	0.531
4	B:38:LEU:O	B:42:LEU:HG	0.527
4	A:224:ALA:HA	A:234:VAL:HG21	0.524
4	A:218:LEU:HD13	A:221:LEU:HD23	0.523
4	A:117:LEU:O	A:121:VAL:HG23	0.521

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:33:HIS:HB2	B:44:LYS:HB3	0.515
4	A:37:LEU:HD13	A:58:ALA:HB2	0.513
4	A:160:TYR:O	A:193:GLY:HA2	0.512
4	A:16:LEU:HD12	A:31:CYS:HB3	0.506
4	A:32:GLU:OE2	B:41:ARG:HD3	0.500
4	A:127:ARG:HD2	A:234:VAL:HG12	0.497
4	A:255:ASN:HB2	A:256:PRO:HD2	0.496
4	A:262:SER:HA	A:394:HIS:ND1	0.496
4	A:61:ALA:HB1	A:66:VAL:HG22	0.495
4	A:189:THR:HB	A:201:ILE:HB	0.491
4	A:132:ARG:HD2	A:149:ASP:O	0.483
4	A:165:GLU:O	A:169:LEU:HG	0.481
4	A:335:THR:HB	A:337:GLN:HG3	0.480
4	A:66:VAL:HG12	A:70:MET:HE3	0.476
4	A:122:ARG:HB3	A:150:ASP:OD2	0.467
4	A:389:SER:O	A:393:ARG:HG3	0.466
4	B:13:ILE:HD11	B:41:ARG:HE	0.459
4	A:104:PHE:HB2	A:441:ILE:HG22	0.458
4	A:11:LEU:HD21	A:48:PHE:HE1	0.456
4	A:213:SER:HB3	A:358:ILE:HG23	0.455
4	A:107:ARG:HD2	A:442:GLU:OE2	0.452
4	A:362:VAL:HG21	B:32:WP9:N41	0.450
4	A:425:THR:HG22	A:429:ALA:HB1	0.446

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:354:THR:HA	A:357:LEU:HD12	0.444
4	A:388:VAL:O	A:392:LEU:HG	0.440
4	A:401:LYS:HZ2	A:404:GLU:CD	0.439
4	B:2:LEU:O	B:5:VAL:HG12	0.436
4	B:6:VAL:HG22	B:46:PHE:CZ	0.435
4	A:159:ARG:HA	A:192:LEU:O	0.433
4	A:470:TYR:CG	A:480:VAL:HG21	0.433
4	A:22:THR:H	A:25:GLU:CG	0.433
4	A:485:ASP:CG	A:488:ARG:HH12	0.432
4	A:11:LEU:HD21	A:48:PHE:CE1	0.428
4	B:46:PHE:CD1	B:68:VAL:HG21	0.428
4	A:218:LEU:HB2	A:221:LEU:HB3	0.424
4	A:106:VAL:HG12	A:200:VAL:HB	0.423
4	A:80:ALA:HA	A:144:GLN:NE2	0.422
4	A:25:GLU:HA	A:26:PRO:HD3	0.421
4	A:372:ASP:OD2	A:375:MET:HE3	0.420
4	A:500:ALA:HA	A:501:PRO:HD3	0.419
4	A:62:THR:O	A:66:VAL:HG23	0.418
4	B:69:GLU:O	B:72:ARG:HG2	0.415
4	A:3:PRO:HG2	A:4:LEU:HD22	0.413
4	A:320:PHE:O	A:324:VAL:HG23	0.413
4	A:481:ARG:HD3	A:485:ASP:OD1	0.409
4	A:152:ALA:O	A:184:PRO:HB3	0.407

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:325:ALA:O	A:329:VAL:HG23	0.407
4	A:29:ASP:C	A:31:CYS:H	0.406
4	A:47:VAL:HG13	A:48:PHE:CD1	0.406
4	B:13:ILE:HG13	B:41:ARG:NH2	0.403
4	A:476:ASP:O	A:480:VAL:HG23	0.402

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	574	534	37	3
2	574	540	32	2
3	574	531	39	4
4	574	530	39	5

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	475	380	46	49
2	475	381	50	44
3	475	374	46	55
4	475	373	49	53

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	7	THR

Model ID	Chain	Residue ID	Residue type
1	A	14	THR
1	A	21	LEU
1	A	29	ASP
1	A	32	GLU
1	A	53	THR
1	A	71	ASP
1	A	72	ASP
1	A	81	SER
1	A	101	ASN
1	A	129	GLU
1	A	134	THR
1	A	156	GLU
1	A	162	ASP
1	A	163	ASP
1	A	167	ASP
1	A	171	HIS
1	A	182	ARG
1	A	218	LEU
1	A	220	GLU
1	A	234	VAL
1	A	264	ASP
1	A	295	THR
1	A	306	ASP

Model ID	Chain	Residue ID	Residue type
1	A	370	GLU
1	A	373	ASP
1	A	400	ASP
1	A	410	ARG
1	A	411	SER
1	A	412	SER
1	A	415	THR
1	A	425	THR
1	A	435	ASP
1	A	442	GLU
1	A	460	ASP
1	A	462	GLU
1	A	467	LEU
1	A	476	ASP
1	A	479	THR
1	A	485	ASP
1	B	4	THR
1	B	7	LEU
1	B	14	SER
1	B	20	THR
1	B	21	THR
1	B	22	THR
1	B	40	SER

Model ID	Chain	Residue ID	Residue type
1	B	52	THR
1	B	56	PHE
2	A	14	THR
2	A	18	SER
2	A	21	LEU
2	A	29	ASP
2	A	32	GLU
2	A	71	ASP
2	A	72	ASP
2	A	81	SER
2	A	101	ASN
2	A	125	LEU
2	A	129	GLU
2	A	134	THR
2	A	156	GLU
2	A	162	ASP
2	A	163	ASP
2	A	182	ARG
2	A	218	LEU
2	A	234	VAL
2	A	295	THR
2	A	370	GLU
2	A	386	GLU

Model ID	Chain	Residue ID	Residue type
2	A	400	ASP
2	A	410	ARG
2	A	411	SER
2	A	412	SER
2	A	415	THR
2	A	421	MET
2	A	425	THR
2	A	435	ASP
2	A	455	LEU
2	A	460	ASP
2	A	462	GLU
2	A	467	LEU
2	A	479	THR
2	A	485	ASP
2	B	4	THR
2	B	7	LEU
2	B	14	SER
2	B	20	THR
2	B	21	THR
2	B	22	THR
2	B	37	GLN
2	B	52	THR
2	B	56	PHE

Model ID	Chain	Residue ID	Residue type
3	A	4	LEU
3	A	7	THR
3	A	14	THR
3	A	21	LEU
3	A	29	ASP
3	A	32	GLU
3	A	53	THR
3	A	71	ASP
3	A	72	ASP
3	A	111	SER
3	A	125	LEU
3	A	129	GLU
3	A	130	VAL
3	A	134	THR
3	A	138	SER
3	A	141	THR
3	A	156	GLU
3	A	162	ASP
3	A	163	ASP
3	A	171	HIS
3	A	173	VAL
3	A	210	ASP
3	A	218	LEU

Model ID	Chain	Residue ID	Residue type
3	A	234	VAL
3	A	264	ASP
3	A	295	THR
3	A	309	GLU
3	A	314	THR
3	A	355	HIS
3	A	370	GLU
3	A	373	ASP
3	A	386	GLU
3	A	400	ASP
3	A	401	LYS
3	A	411	SER
3	A	412	SER
3	A	415	THR
3	A	425	THR
3	A	435	ASP
3	A	455	LEU
3	A	459	ARG
3	A	460	ASP
3	A	462	GLU
3	A	479	THR
3	A	485	ASP
3	B	7	LEU

Model ID	Chain	Residue ID	Residue type
3	B	14	SER
3	B	20	THR
3	B	21	THR
3	B	22	THR
3	B	40	SER
3	B	52	THR
3	B	53	GLU
3	B	60	THR
3	B	71	SER
4	A	7	THR
4	A	14	THR
4	A	18	SER
4	A	21	LEU
4	A	29	ASP
4	A	53	THR
4	A	71	ASP
4	A	72	ASP
4	A	111	SER
4	A	125	LEU
4	A	129	GLU
4	A	134	THR
4	A	138	SER
4	A	141	THR

Model ID	Chain	Residue ID	Residue type
4	A	156	GLU
4	A	162	ASP
4	A	163	ASP
4	A	171	HIS
4	A	173	VAL
4	A	210	ASP
4	A	218	LEU
4	A	220	GLU
4	A	234	VAL
4	A	264	ASP
4	A	295	THR
4	A	309	GLU
4	A	314	THR
4	A	370	GLU
4	A	373	ASP
4	A	386	GLU
4	A	400	ASP
4	A	411	SER
4	A	412	SER
4	A	415	THR
4	A	425	THR
4	A	435	ASP
4	A	455	LEU

Model ID	Chain	Residue ID	Residue type
4	A	459	ARG
4	A	460	ASP
4	A	462	GLU
4	A	467	LEU
4	A	479	THR
4	A	485	ASP
4	B	7	LEU
4	B	14	SER
4	B	20	THR
4	B	21	THR
4	B	22	THR
4	B	45	ILE
4	B	52	THR
4	B	53	GLU
4	B	60	THR
4	B	71	SER

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.

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