Integrative Structure Validation Report

July 22, 2024 - 04:43 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	9A1R
PDB-Dev ID	PDBDEV_00000099
Structure Title	INTEGRATIVE STRUCTURE OF BTG2 IN COMPLEX WITH RRM1-2 OF PABPC1
Structure Authors	Ameerul, A.; Almasmoum, H.; Pavanello, L.; Dominguez, C.; Winkler, G.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

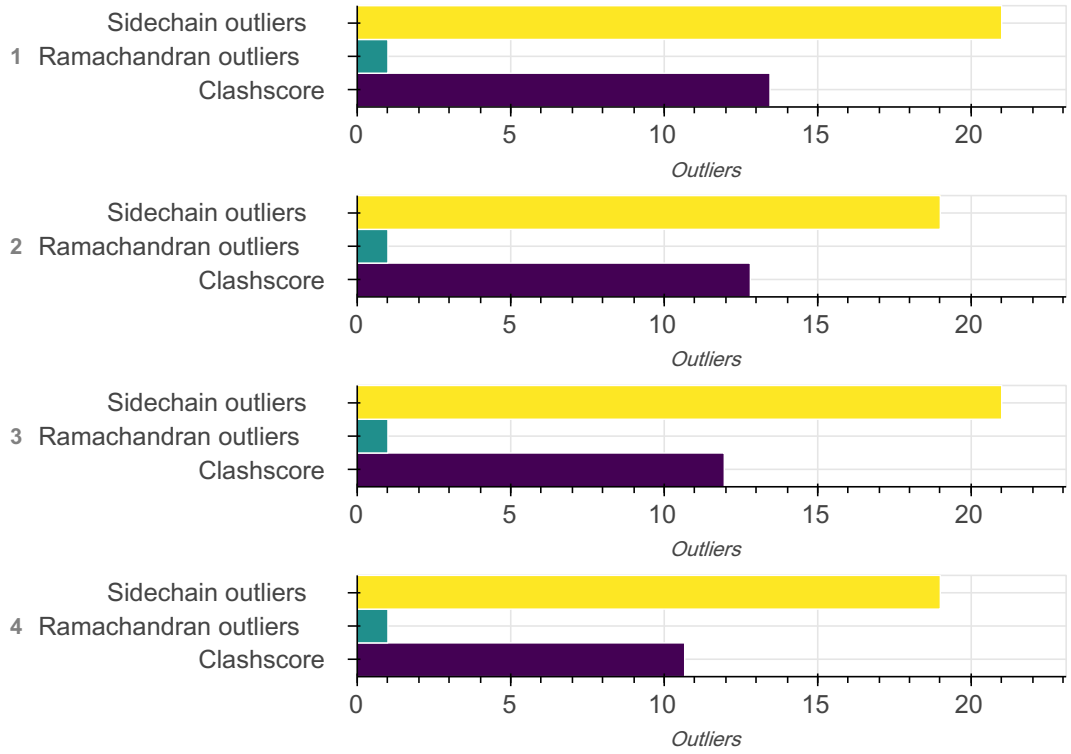
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 4 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 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	POLY(A) BINDING PROTEIN CYTOPLASMIC 1	A	A	175
1	2	2	PROTEIN BTG2	B	B	121
2	1	1	POLY(A) BINDING PROTEIN CYTOPLASMIC 1	A	A	175

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	2	2	PROTEIN BTG2	B	B	121
3	1	1	POLY(A) BINDING PROTEIN CYTOPLASMIC 1	A	A	175
3	2	2	PROTEIN BTG2	B	B	121
4	1	1	POLY(A) BINDING PROTEIN CYTOPLASMIC 1	A	A	175
4	2	2	PROTEIN BTG2	B	B	121

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	Experimental model	PDB	4F02
2	Experimental model	PDB	3DJU
3	NMR data	BMRB	50526

Representation

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

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-175
B	-	1-121

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	Rigid-body minimization in HADDOCK (it0)	Rigid-body minimization	None	1000	False	False
2	1	Semi-flexible SA in HADDOCK (it1)	Simulated annealing	None	200	False	False
3	1	Water refinement in HADDOCK (itw)	Refinement	None	200	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.4	Molecular docking	http://haddock.science.uu.nl/services/HADDOCK/

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 2144 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--H	0.97	0.86	9

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE21	0.97	0.86	3
ND2--HD22	0.97	0.86	1
N--H	0.98	0.86	1015
ND2--HD22	0.98	0.86	39
NE2--HE21	0.98	0.86	37
NE1--HE1	0.98	0.86	11
NE2--HE22	0.98	0.86	39
ND2--HD21	0.98	0.86	27
NE2--HE2	0.98	0.86	24
OG--HG	0.96	0.84	57
OH--HH	0.96	0.84	33
NE--HE	0.98	0.86	58
ND1--HD1	0.98	0.86	8
OG1--HG1	0.96	0.84	18
SG--HG	1.32	1.20	15
N--H	0.99	0.86	96
SG--HG	1.33	1.20	9
NE1--HE1	0.99	0.86	1
OG--HG	0.97	0.84	28
OH--HH	0.97	0.84	9
OG1--HG1	0.97	0.84	14
ND2--HD21	0.99	0.86	10
NE2--HE2	0.99	0.86	4

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE--HE	0.99	0.86	18
NE2--HE22	0.99	0.86	1
ND2--HD21	1.00	0.86	3
OG--HG	0.98	0.84	11
OH--HH	0.98	0.84	2
OG1--HG1	0.98	0.84	4
NE--HE	1.00	0.86	4
NZ--HZ2	1.03	0.89	7
NZ--HZ3	1.04	0.89	55
NZ--HZ1	1.04	0.89	68
NZ--HZ2	1.04	0.89	59
NZ--HZ2	1.05	0.89	6
NZ--HZ3	1.05	0.89	17
NZ--HZ1	1.05	0.89	4
NH1--HH11	1.04	0.86	48
NH2--HH21	1.04	0.86	57
NH1--HH12	1.04	0.86	47
NH2--HH22	1.04	0.86	45
NH1--HH12	1.05	0.86	23
NH1--HH11	1.05	0.86	28
NH2--HH22	1.05	0.86	20
NH2--HH21	1.05	0.86	15
NH2--HH21	1.06	0.86	8

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH1--HH12	1.06	0.86	10
NH2--HH22	1.06	0.86	15
NH1--HH11	1.06	0.86	4

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 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	13.45	63
2	12.81	60
3	11.96	56
4	10.67	50

All 229 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:10:HIS:HB3	A:13:VAL:HG23	0.743
1	B:39:ALA:HA	B:42:GLU:OE2	0.679
1	A:5:TYR:HD2	A:76:MET:HB2	0.674
1	B:3:MET:HE1	B:45:LYS:HA	0.668
1	A:91:ASN:HA	A:135:HIS:HA	0.661
1	A:60:LEU:O	A:64:ASN:HB2	0.628
1	A:40:ARG:HH22	B:118:GLU:HG2	0.620
1	B:106:ARG:NH1	B:109:GLU:HA	0.618
1	A:15:GLU:HG2	A:33:VAL:HG23	0.595

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:107:ILE:O	B:111:GLY:HA3	0.590
1	A:68:ILE:HD12	A:73:VAL:HG11	0.581
1	A:94:ILE:HG23	A:161:VAL:HG22	0.548
1	B:64:ILE:HD12	B:94:LEU:HD23	0.548
1	A:35:ARG:HG2	A:42:SER:HA	0.545
1	A:140:GLU:CD	A:140:GLU:H	0.545
1	B:7:ILE:HG22	B:37:GLN:HG2	0.538
1	A:9:LEU:HD23	A:73:VAL:HG12	0.532
1	A:15:GLU:HG2	A:33:VAL:CG2	0.531
1	B:32:PHE:HB2	B:79:ILE:HD13	0.524
1	A:21:LYS:HG2	A:68:ILE:HD11	0.521
1	A:87:SER:HB2	A:89:VAL:HG23	0.519
1	A:144:ARG:HA	A:147:GLU:OE1	0.513
1	A:3:SER:HB2	A:78:SER:HB2	0.512
1	B:11:VAL:HG21	B:37:GLN:HG3	0.512
1	A:33:VAL:HG22	A:46:ALA:HB2	0.511
1	A:122:VAL:HG21	A:131:TYR:CE2	0.502
1	A:74:ARG:HD2	A:120:LYS:HB2	0.488
1	B:75:VAL:HA	B:78:GLN:OE1	0.487
1	B:101:TYR:O	B:118:GLU:HA	0.487
1	A:122:VAL:HG21	A:131:TYR:CZ	0.485
1	A:140:GLU:HA	A:143:GLU:OE1	0.485
1	B:68:MET:HE3	B:86:LEU:HB3	0.478

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:31:ILE:O	B:114:CYS:HA	0.478
1	B:106:ARG:HH12	B:109:GLU:HA	0.471
1	A:22:PHE:HB3	A:50:PHE:CZ	0.470
1	B:36:LEU:O	B:40:LEU:HG	0.469
1	A:15:GLU:OE1	A:32:ARG:HA	0.461
1	A:97:LEU:O	A:130:GLY:HA2	0.461
1	A:19:TYR:HE1	B:111:GLY:HA2	0.461
1	A:97:LEU:HD23	A:159:VAL:HG11	0.460
1	B:49:PHE:O	B:100:PRO:HG2	0.458
1	A:92:ILE:HG23	A:142:ALA:HB1	0.454
1	A:27:PRO:HD2	A:55:ASP:OD2	0.452
1	A:76:MET:SD	A:118:SER:HB2	0.451
1	A:22:PHE:HB3	A:50:PHE:HZ	0.449
1	A:140:GLU:O	A:144:ARG:HG3	0.447
1	B:94:LEU:HD13	B:107:ILE:HG12	0.444
1	B:41:THR:O	B:45:LYS:HB2	0.443
1	A:8:ASP:OD1	A:74:ARG:HD3	0.438
1	A:71:LYS:HB3	A:71:LYS:HE2	0.436
1	A:20:GLU:H	A:20:GLU:HG2	0.431
1	A:23:SER:HB3	A:24:PRO:HD3	0.430
1	B:60:ARG:HH21	B:99:ASP:CG	0.428
1	B:11:VAL:HG13	B:36:LEU:HD23	0.427
1	A:36:ASP:O	A:40:ARG:HA	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:120:ALA:HA	B:121:PRO:HD3	0.417
1	A:52:GLN:HB2	A:55:ASP:OD2	0.411
1	A:123:CYS:HA	A:127:GLY:O	0.409
1	A:3:SER:HB2	A:78:SER:CB	0.407
1	A:15:GLU:CD	B:114:CYS:HB3	0.405
1	A:170:ARG:HH21	A:174:LEU:HD21	0.403
1	B:63:ARG:HD3	B:95:THR:HG23	0.403
1	B:76:ALA:HB1	B:81:LEU:HB2	0.401
2	B:104:SER:HB3	B:115:VAL:HG22	0.789
2	A:10:HIS:HB3	A:13:VAL:HG23	0.715
2	A:15:GLU:HG2	A:33:VAL:HG23	0.706
2	B:39:ALA:HA	B:42:GLU:OE2	0.694
2	B:3:MET:HE1	B:45:LYS:HA	0.693
2	A:21:LYS:HG2	A:68:ILE:HD11	0.688
2	A:60:LEU:O	A:64:ASN:HB2	0.658
2	A:91:ASN:HA	A:135:HIS:HA	0.657
2	A:31:ILE:O	B:114:CYS:HA	0.624
2	A:5:TYR:HD2	A:76:MET:HB2	0.622
2	A:68:ILE:HD12	A:73:VAL:HG11	0.595
2	A:35:ARG:HG2	A:42:SER:HA	0.592
2	A:33:VAL:HG22	A:46:ALA:HB2	0.581
2	B:7:ILE:HG22	B:37:GLN:HG2	0.567
2	B:32:PHE:HB2	B:79:ILE:HD13	0.551

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:106:ARG:NH1	B:109:GLU:HA	0.544
2	A:140:GLU:CD	A:140:GLU:H	0.543
2	A:94:ILE:HG23	A:161:VAL:HG22	0.538
2	A:87:SER:HB2	A:89:VAL:HG23	0.522
2	A:9:LEU:HD23	A:73:VAL:HG12	0.519
2	A:12:ASP:CB	A:69:LYS:HE2	0.517
2	A:144:ARG:HA	A:147:GLU:OE1	0.515
2	B:93:GLU:HB3	B:108:GLY:HA2	0.503
2	A:122:VAL:HG21	A:131:TYR:CE2	0.498
2	B:11:VAL:HG21	B:37:GLN:HG3	0.497
2	B:75:VAL:HA	B:78:GLN:OE1	0.497
2	A:122:VAL:HG21	A:131:TYR:CZ	0.487
2	B:64:ILE:HD12	B:94:LEU:HD23	0.487
2	A:3:SER:HB2	A:78:SER:HB2	0.486
2	A:74:ARG:HD2	A:120:LYS:HD2	0.484
2	A:140:GLU:HA	A:143:GLU:OE1	0.484
2	A:3:SER:HB2	A:78:SER:CB	0.481
2	A:12:ASP:HB3	A:69:LYS:HE2	0.481
2	A:36:ASP:O	A:40:ARG:HA	0.474
2	A:74:ARG:HD2	A:120:LYS:HB2	0.473
2	B:103:VAL:HB	B:117:TYR:HB3	0.473
2	B:36:LEU:O	B:40:LEU:HG	0.470
2	B:68:MET:HE3	B:86:LEU:HB3	0.470

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:32:ARG:NH2	B:118:GLU:HG2	0.468
2	B:76:ALA:HB1	B:81:LEU:HB2	0.464
2	A:97:LEU:HD23	A:159:VAL:HG11	0.463
2	B:93:GLU:CB	B:108:GLY:HA2	0.463
2	A:97:LEU:O	A:130:GLY:HA2	0.462
2	A:76:MET:SD	A:118:SER:HB2	0.456
2	A:92:ILE:HG23	A:142:ALA:HB1	0.454
2	A:15:GLU:CD	B:114:CYS:HB3	0.448
2	B:41:THR:O	B:45:LYS:HB2	0.448
2	B:101:TYR:O	B:118:GLU:HA	0.445
2	A:140:GLU:O	A:144:ARG:HG3	0.444
2	B:101:TYR:CZ	B:121:PRO:HA	0.437
2	A:37:MET:HB3	B:119:GLU:OE2	0.433
2	B:49:PHE:O	B:100:PRO:HG2	0.433
2	A:23:SER:HB3	A:24:PRO:HD3	0.431
2	B:39:ALA:HB1	B:74:ARG:NH2	0.421
2	B:107:ILE:O	B:111:GLY:HA3	0.416
2	A:123:CYS:HA	A:127:GLY:O	0.412
2	A:52:GLN:HA	A:53:PRO:HD3	0.405
2	A:147:GLU:HG2	A:148:LYS:HG3	0.404
2	B:11:VAL:HG13	B:36:LEU:HD23	0.404
2	A:170:ARG:HH21	A:174:LEU:HD21	0.401
3	B:3:MET:HE1	B:45:LYS:HA	0.732

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:10:HIS:HB3	A:13:VAL:HG23	0.688
3	B:103:VAL:HB	B:117:TYR:HB3	0.671
3	B:39:ALA:HA	B:42:GLU:OE2	0.666
3	A:91:ASN:HA	A:135:HIS:HA	0.654
3	A:5:TYR:HD2	A:76:MET:HB2	0.653
3	B:106:ARG:HG3	B:113:ILE:HD13	0.635
3	B:106:ARG:NH2	B:109:GLU:HA	0.627
3	A:60:LEU:O	A:64:ASN:HB2	0.626
3	A:15:GLU:HG3	A:33:VAL:HG23	0.615
3	A:11:PRO:HA	A:42:SER:HB3	0.592
3	A:35:ARG:HG2	A:42:SER:HA	0.584
3	B:93:GLU:HB2	B:108:GLY:HA2	0.576
3	A:17:MET:SD	A:69:LYS:HD2	0.571
3	A:74:ARG:HD2	A:120:LYS:HB2	0.559
3	B:7:ILE:HG22	B:37:GLN:HG2	0.543
3	B:32:PHE:HB2	B:79:ILE:HD13	0.540
3	A:140:GLU:CD	A:140:GLU:H	0.539
3	A:68:ILE:HD12	A:73:VAL:HG11	0.538
3	A:94:ILE:HG23	A:161:VAL:HG22	0.534
3	B:68:MET:HE3	B:86:LEU:HB3	0.518
3	A:52:GLN:HB2	A:55:ASP:OD2	0.517
3	A:3:SER:HB2	A:78:SER:HB2	0.516
3	A:87:SER:HB2	A:89:VAL:HG23	0.511

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:31:ILE:O	B:114:CYS:HA	0.511
3	A:122:VAL:HG21	A:131:TYR:CE2	0.510
3	A:144:ARG:HA	A:147:GLU:OE1	0.492
3	B:75:VAL:HA	B:78:GLN:OE1	0.491
3	A:21:LYS:HG2	A:68:ILE:HD11	0.487
3	A:122:VAL:HG21	A:131:TYR:CZ	0.486
3	B:107:ILE:O	B:111:GLY:HA3	0.483
3	A:3:SER:HB2	A:78:SER:CB	0.481
3	A:140:GLU:HA	A:143:GLU:OE1	0.478
3	A:10:HIS:O	A:13:VAL:HB	0.468
3	B:11:VAL:HG21	B:37:GLN:HG3	0.467
3	B:76:ALA:HB1	B:81:LEU:HB2	0.466
3	A:76:MET:SD	A:118:SER:HB2	0.463
3	A:27:PRO:HD2	A:55:ASP:OD2	0.460
3	A:140:GLU:O	A:144:ARG:HG3	0.452
3	A:97:LEU:O	A:130:GLY:HA2	0.451
3	B:60:ARG:HH21	B:99:ASP:CG	0.445
3	A:36:ASP:O	A:40:ARG:HA	0.443
3	A:92:ILE:HG23	A:142:ALA:HB1	0.442
3	B:106:ARG:HH21	B:109:GLU:HA	0.441
3	B:36:LEU:O	B:40:LEU:HG	0.438
3	A:97:LEU:HD23	A:159:VAL:HG11	0.437
3	B:41:THR:O	B:45:LYS:HB2	0.432

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:9:LEU:HD23	A:73:VAL:HG12	0.431
3	B:49:PHE:O	B:100:PRO:HG2	0.421
3	A:32:ARG:HG3	B:115:VAL:HB	0.416
3	A:23:SER:HB3	A:24:PRO:HD3	0.414
3	A:123:CYS:HA	A:127:GLY:O	0.413
3	A:95:LYS:HB3	A:95:LYS:HE2	0.412
3	A:71:LYS:HB3	A:71:LYS:HE2	0.404
3	B:3:MET:HB3	B:48:TRP:CE2	0.401
3	B:11:VAL:HG13	B:36:LEU:HD23	0.400
4	B:3:MET:HE1	B:45:LYS:HA	0.741
4	A:5:TYR:HD2	A:76:MET:HB2	0.740
4	A:10:HIS:HB3	A:13:VAL:HG23	0.670
4	A:91:ASN:HA	A:135:HIS:HA	0.628
4	B:39:ALA:HA	B:42:GLU:OE2	0.627
4	B:107:ILE:O	B:111:GLY:HA3	0.597
4	A:21:LYS:HG2	A:68:ILE:HD11	0.594
4	A:60:LEU:O	A:64:ASN:HB2	0.590
4	A:33:VAL:HG22	A:46:ALA:HB2	0.588
4	A:9:LEU:HD22	A:13:VAL:HG11	0.575
4	A:122:VAL:HG21	A:131:TYR:CE2	0.561
4	B:64:ILE:HD12	B:94:LEU:HD23	0.551
4	A:15:GLU:HG3	A:33:VAL:HG23	0.547
4	A:76:MET:SD	A:118:SER:HB2	0.547

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	B:7:ILE:HG22	B:37:GLN:HG2	0.544
4	A:140:GLU:CD	A:140:GLU:H	0.534
4	B:32:PHE:HB2	B:79:ILE:HD13	0.532
4	B:106:ARG:NH2	B:109:GLU:HA	0.524
4	B:101:TYR:CZ	B:121:PRO:HA	0.509
4	A:74:ARG:HD2	A:120:LYS:HB2	0.508
4	B:94:LEU:HD13	B:107:ILE:HG12	0.502
4	A:122:VAL:HG21	A:131:TYR:CZ	0.501
4	A:94:ILE:HG23	A:161:VAL:HG22	0.498
4	A:68:ILE:HD12	A:73:VAL:HG11	0.491
4	A:87:SER:HB2	A:89:VAL:HG23	0.490
4	B:28:ARG:HD2	B:79:ILE:O	0.486
4	A:11:PRO:HA	A:42:SER:HB3	0.464
4	A:140:GLU:O	A:144:ARG:HG3	0.463
4	A:23:SER:HB3	A:24:PRO:HD3	0.453
4	B:75:VAL:HA	B:78:GLN:OE1	0.453
4	A:27:PRO:HD2	A:55:ASP:OD2	0.450
4	A:122:VAL:HG22	A:131:TYR:O	0.449
4	B:11:VAL:HG21	B:37:GLN:HG3	0.449
4	B:68:MET:HE3	B:86:LEU:HB3	0.447
4	B:60:ARG:HH21	B:99:ASP:CG	0.440
4	B:3:MET:HB3	B:48:TRP:CE2	0.436
4	A:36:ASP:O	A:40:ARG:HA	0.434

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	B:93:GLU:HB2	B:108:GLY:HA2	0.432
4	A:15:GLU:HG2	A:32:ARG:HA	0.430
4	B:38:GLU:O	B:42:GLU:HG3	0.430
4	A:97:LEU:O	A:130:GLY:HA2	0.427
4	B:120:ALA:HA	B:121:PRO:HD3	0.423
4	B:101:TYR:O	B:118:GLU:HA	0.422
4	A:10:HIS:ND1	A:12:ASP:HB2	0.416
4	A:27:PRO:HB2	A:51:GLN:CD	0.413
4	B:76:ALA:HB1	B:81:LEU:HB2	0.413
4	A:52:GLN:HA	A:53:PRO:HD3	0.412
4	A:9:LEU:HD23	A:73:VAL:HG12	0.404
4	A:71:LYS:HB3	A:71:LYS:HE2	0.403
4	A:123:CYS:HA	A:127:GLY:O	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	292	277	14	1
2	292	276	15	1
3	292	279	12	1
4	292	277	14	1

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	255	205	29	21
2	255	204	32	19
3	255	204	30	21
4	255	203	33	19

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	8	ASP
1	A	20	GLU
1	A	62	THR
1	A	87	SER
1	A	94	ILE
1	A	102	ASP
1	A	138	THR
1	A	140	GLU
1	A	147	GLU
1	A	171	GLU
1	B	25	SER
1	B	30	LYS
1	B	41	THR
1	B	54	SER
1	B	92	SER
1	B	95	THR
1	B	96	LEU

Model ID	Chain	Residue ID	Residue type
1	B	102	GLU
1	B	104	SER
1	B	116	LEU
1	B	119	GLU
2	A	62	THR
2	A	87	SER
2	A	102	ASP
2	A	138	THR
2	A	140	GLU
2	A	147	GLU
2	A	171	GLU
2	B	18	LEU
2	B	20	THR
2	B	25	SER
2	B	30	LYS
2	B	41	THR
2	B	54	SER
2	B	92	SER
2	B	95	THR
2	B	96	LEU
2	B	104	SER
2	B	112	SER
2	B	118	GLU

Model ID	Chain	Residue ID	Residue type
3	A	14	THR
3	A	32	ARG
3	A	62	THR
3	A	87	SER
3	A	102	ASP
3	A	138	THR
3	A	140	GLU
3	A	147	GLU
3	A	171	GLU
3	B	18	LEU
3	B	19	ARG
3	B	25	SER
3	B	30	LYS
3	B	41	THR
3	B	54	SER
3	B	92	SER
3	B	96	LEU
3	B	102	GLU
3	B	104	SER
3	B	112	SER
3	B	116	LEU
4	A	12	ASP
4	A	28	ILE

Model ID	Chain	Residue ID	Residue type
4	A	30	SER
4	A	32	ARG
4	A	102	ASP
4	A	138	THR
4	A	140	GLU
4	A	147	GLU
4	B	19	ARG
4	B	25	SER
4	B	30	LYS
4	B	41	THR
4	B	54	SER
4	B	92	SER
4	B	96	LEU
4	B	102	GLU
4	B	104	SER
4	B	110	ASP
4	B	116	LEU

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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