Integrative Structure Validation Report

July 22, 2024 - 04:24 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	9A1A
PDB-Dev ID	PDBDEV_00000082
Structure Title	The ensemble structure of alpha-synuclein monomer
Structure Authors	Chen J; Zaer S; Drori P; Zamel J; Joron K; Kalisman N; Lerner E; Dokholyan NV

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

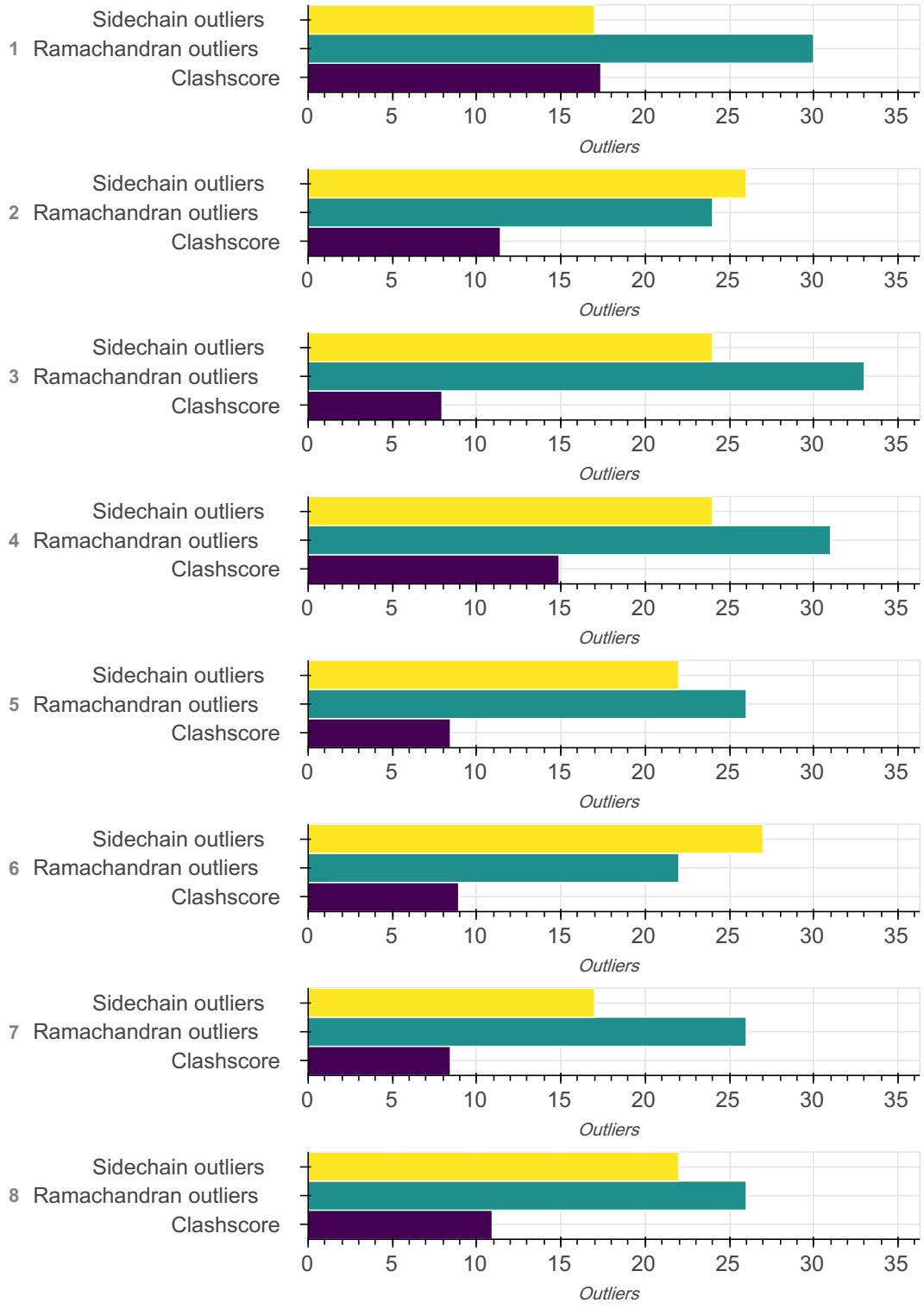
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 8 distinct ensemble(s).

Summary

This entry consists of 8 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 8 unique types of models in this entry.These models are titled cluster 1/cluster1_centroid, cluster 2/cluster2_centroid, cluster 3/cluster3_centroid, cluster 4/cluster4_centroid, cluster 5/cluster5_centroid, cluster 6/cluster6_centroid, cluster 7/cluster7_centroid, cluster 8/cluster8_centroid respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	alpha-synuclein	A	A	140
2	1	1	alpha-synuclein	A	A	140
3	1	1	alpha-synuclein	A	A	140
4	1	1	alpha-synuclein	A	A	140
5	1	1	alpha-synuclein	A	A	140
6	1	1	alpha-synuclein	A	A	140
7	1	1	alpha-synuclein	A	A	140
8	1	1	alpha-synuclein	A	A	140

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	Other	File	10.1016/j.jmb.2010.11.011

Representation

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

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-140

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	Discrete molecular dynamics simulations	None	30303	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	piDMD	Not available	model building	http://www.moleculesinaction.com/home.html
2	TTClust	Not available	structure clustering	https://github.com/tubiana/TTClust

Data quality

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 1448 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

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ2	0.98	0.89	30
NZ--HZ1	0.98	0.89	26
NZ--HZ3	0.98	0.89	25
NZ--HZ3	0.99	0.89	32
NZ--HZ1	0.99	0.89	41
NZ--HZ2	0.99	0.89	38
NZ--HZ2	1.00	0.89	26
NZ--HZ3	1.00	0.89	46
NZ--HZ1	1.00	0.89	25
NZ--HZ3	1.01	0.89	12
NZ--HZ2	1.01	0.89	20
NZ--HZ1	1.01	0.89	21
N--H	0.98	0.86	70
N--H	0.99	0.86	184
NZ--HZ1	1.02	0.89	6
NZ--HZ3	1.02	0.89	3
NZ--HZ2	1.02	0.89	4
ND1--HD1	0.99	0.86	2
N--H	1.00	0.86	291
ND1--HD1	1.00	0.86	2
N--H	1.01	0.86	349
ND1--HD1	1.01	0.86	1
N--H	1.02	0.86	186

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND1--HD1	1.02	0.86	3
NZ--HZ2	1.73	0.89	1
NZ--HZ3	1.73	0.89	1
NZ--HZ2	1.77	0.89	1
NZ--HZ1	1.77	0.89	1
NZ--HZ3	1.81	0.89	1

Standard geometry: angle outliers

There are 24 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
CD-CE-NZ	111.90	86.45	1
CA-CB-CG1	110.40	117.71	1
CA-CB-CG	112.60	116.81	1
CA-CB-CG	112.60	116.76	1
CA-CB-CG2	110.40	117.38	1
CA-CB-CG	112.60	116.70	1
CE-NZ-HZ1	76.86	110.00	1
CE-NZ-HZ3	76.23	110.00	1
CE-NZ-HZ2	76.04	110.00	1
CE-NZ-HZ2	74.47	110.00	1
CE-NZ-HZ3	73.39	110.00	1
CE-NZ-HZ2	72.17	110.00	1
CE-NZ-HZ3	70.73	110.00	1
HZ1-NZ-HZ2	69.47	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CE-NZ-HZ1	70.14	110.00	1
HZ2-NZ-HZ3	68.11	109.00	1
HZ2-NZ-HZ3	67.05	109.00	1
HZ2-NZ-HZ3	66.94	109.00	1
HZ1-NZ-HZ3	66.63	109.00	1
HZ1-NZ-HZ2	66.41	109.00	1
HZ1-NZ-HZ3	66.41	109.00	1
HZ2-NZ-HZ3	65.07	109.00	1
HZ1-NZ-HZ2	63.80	109.00	1
HZ1-NZ-HZ3	62.82	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	17.37	35
2	11.41	23
3	7.94	16
4	14.89	30
5	8.44	17
6	8.93	18
7	8.44	17
8	10.92	22

All 178 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:21:LYS:CE	A:21:LYS:NZ	1.157
1	A:18:ALA:HB2	A:49:VAL:HG13	0.948
1	A:30:ALA:HB1	A:99:GLN:HB2	0.814
1	A:19:ALA:HB1	A:34:LYS:HE3	0.787
1	A:4:PHE:HB2	A:70:VAL:HG23	0.767
1	A:21:LYS:CD	A:21:LYS:NZ	0.741
1	A:49:VAL:HG23	A:87:SER:HB2	0.723
1	A:4:PHE:HD1	A:71:VAL:HA	0.702
1	A:30:ALA:HB3	A:95:VAL:HG12	0.694
1	A:11:ALA:HA	A:56:ALA:HA	0.660
1	A:130:GLU:HA	A:134:GLN:HB2	0.651
1	A:9:SER:HB3	A:76:ALA:HB1	0.650
1	A:4:PHE:HE1	A:72:THR:HG22	0.647
1	A:15:VAL:HG22	A:138:PRO:HG2	0.636
1	A:95:VAL:HA	A:98:ASP:HB2	0.635
1	A:52:VAL:HG11	A:136:TYR:HE2	0.604
1	A:19:ALA:HB3	A:24:GLN:HB2	0.600
1	A:87:SER:HB3	A:95:VAL:HG22	0.582
1	A:52:VAL:HG21	A:88:ILE:HD11	0.554
1	A:58:LYS:HD2	A:67:GLY:HA2	0.546
1	A:62:GLN:HG3	A:63:VAL:HG22	0.544
1	A:130:GLU:HA	A:134:GLN:CB	0.519
1	A:30:ALA:CB	A:95:VAL:HG12	0.514

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:56:ALA:HB3	A:79:GLN:H	0.511
1	A:49:VAL:HG21	A:113:LEU:HD11	0.501
1	A:91:ALA:HB1	A:96:LYS:HB2	0.488
1	A:77:VAL:HG22	A:79:GLN:HG3	0.475
1	A:9:SER:HB3	A:76:ALA:CB	0.469
1	A:52:VAL:HG11	A:136:TYR:CE2	0.459
1	A:21:LYS:HD2	A:21:LYS:NZ	0.458
1	A:33:THR:HG22	A:38:LEU:HB2	0.454
1	A:49:VAL:CG2	A:87:SER:HB2	0.448
1	A:119:ASP:HA	A:120:PRO:HD2	0.441
1	A:38:LEU:HD22	A:48:VAL:CG2	0.412
1	A:15:VAL:O	A:52:VAL:HG12	0.401
2	A:119:ASP:HB2	A:125:TYR:HD1	0.886
2	A:1:MET:HE3	A:6:LYS:HB3	0.849
2	A:99:GLN:HG3	A:112:ILE:HD11	0.670
2	A:16:VAL:HA	A:22:THR:HG22	0.619
2	A:60:LYS:HB3	A:95:VAL:HG21	0.606
2	A:19:ALA:HB3	A:22:THR:HB	0.593
2	A:21:LYS:HB2	A:90:ALA:HB3	0.592
2	A:88:ILE:HA	A:93:GLY:HA2	0.554
2	A:55:VAL:HG23	A:95:VAL:HG23	0.546
2	A:72:THR:HG22	A:94:PHE:HE1	0.536
2	A:119:ASP:HB2	A:125:TYR:CD1	0.517

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:70:VAL:HG12	A:80:LYS:HG3	0.482
2	A:42:SER:HB2	A:45:LYS:HB3	0.448
2	A:49:VAL:HG22	A:88:ILE:HG23	0.444
2	A:8:LEU:HA	A:8:LEU:HD23	0.433
2	A:94:PHE:CD2	A:95:VAL:HG12	0.432
2	A:109:GLN:HE21	A:114:GLU:HG2	0.428
2	A:8:LEU:HD11	A:120:PRO:HG3	0.425
2	A:59:THR:CG2	A:62:GLN:HG2	0.423
2	A:127:MET:HA	A:128:PRO:HD3	0.420
2	A:42:SER:OG	A:46:GLU:HB2	0.419
2	A:35:GLU:O	A:44:THR:HG23	0.403
2	A:70:VAL:HA	A:80:LYS:HG3	0.400
3	A:18:ALA:HB1	A:22:THR:HG22	0.704
3	A:120:PRO:HA	A:124:ALA:HB3	0.687
3	A:15:VAL:HG22	A:134:GLN:HG2	0.649
3	A:95:VAL:HG12	A:97:LYS:HG3	0.621
3	A:55:VAL:HG21	A:88:ILE:HG22	0.602
3	A:1:MET:HE3	A:6:LYS:HB3	0.573
3	A:64:THR:HG23	A:112:ILE:HG23	0.566
3	A:108:PRO:HG2	A:120:PRO:HB3	0.536
3	A:44:THR:HG23	A:87:SER:HB2	0.528
3	A:12:LYS:HA	A:37:VAL:HG21	0.503
3	A:11:ALA:HB1	A:12:LYS:HE2	0.498

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:12:LYS:HG2	A:29:ALA:HB1	0.473
3	A:70:VAL:HG23	A:113:LEU:HD21	0.426
3	A:116:MET:HA	A:117:PRO:HD3	0.426
3	A:19:ALA:HB1	A:127:MET:CB	0.409
3	A:43:LYS:HB2	A:43:LYS:HE3	0.402
4	A:40:VAL:HG12	A:47:GLY:HA2	0.949
4	A:117:PRO:HG2	A:128:PRO:HA	0.728
4	A:15:VAL:HG11	A:82:VAL:HG22	0.638
4	A:108:PRO:HA	A:112:ILE:HB	0.632
4	A:131:GLU:HG2	A:135:ASP:HB2	0.617
4	A:8:LEU:HD12	A:128:PRO:HB3	0.610
4	A:91:ALA:HB3	A:118:VAL:HB	0.579
4	A:8:LEU:HD13	A:16:VAL:HB	0.544
4	A:74:VAL:HG12	A:138:PRO:HG3	0.541
4	A:23:LYS:HE3	A:64:THR:HG22	0.537
4	A:103:ASN:HB2	A:110:GLU:HG3	0.532
4	A:102:LYS:HB2	A:110:GLU:HB2	0.517
4	A:30:ALA:HB3	A:48:VAL:HG11	0.500
4	A:8:LEU:HD21	A:88:ILE:HD12	0.496
4	A:94:PHE:HD2	A:114:GLU:HB2	0.494
4	A:4:PHE:CE2	A:119:ASP:HB2	0.486
4	A:4:PHE:HB3	A:8:LEU:HB2	0.484
4	A:15:VAL:HG13	A:16:VAL:HG13	0.473

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:11:ALA:HB3	A:15:VAL:HG23	0.468
4	A:55:VAL:HA	A:60:LYS:HA	0.456
4	A:5:MET:HE1	A:87:SER:HB3	0.455
4	A:102:LYS:HE2	A:114:GLU:HG3	0.454
4	A:38:LEU:HA	A:38:LEU:HD23	0.449
4	A:4:PHE:CD1	A:8:LEU:HD22	0.445
4	A:116:MET:HB2	A:116:MET:HE2	0.435
4	A:8:LEU:CD1	A:16:VAL:HB	0.431
4	A:23:LYS:HA	A:23:LYS:HD2	0.407
4	A:30:ALA:CB	A:48:VAL:HG11	0.403
4	A:74:VAL:CG1	A:138:PRO:HG3	0.402
4	A:15:VAL:CG1	A:82:VAL:HG22	0.400
5	A:4:PHE:HB3	A:7:GLY:HA2	0.717
5	A:17:ALA:HA	A:21:LYS:HD3	0.613
5	A:8:LEU:HD21	A:74:VAL:HG21	0.583
5	A:15:VAL:HG21	A:59:THR:HG21	0.566
5	A:66:VAL:HG23	A:70:VAL:HB	0.549
5	A:26:VAL:HG21	A:37:VAL:HG21	0.540
5	A:91:ALA:HB2	A:114:GLU:HB2	0.540
5	A:26:VAL:HG11	A:37:VAL:HG11	0.519
5	A:1:MET:HE1	A:8:LEU:HD23	0.515
5	A:83:GLU:HB3	A:89:ALA:HB3	0.509
5	A:37:VAL:HG13	A:48:VAL:HB	0.487

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:108:PRO:HA	A:114:GLU:HG3	0.487
5	A:136:TYR:CD1	A:137:GLU:HG3	0.448
5	A:14:GLY:HA2	A:18:ALA:HB3	0.430
5	A:80:LYS:HB3	A:96:LYS:HG3	0.430
5	A:137:GLU:HA	A:138:PRO:C	0.401
5	A:79:GLN:HB2	A:94:PHE:HD1	0.400
6	A:70:VAL:HG22	A:94:PHE:HE1	0.695
6	A:94:PHE:HE2	A:100:LEU:HD22	0.678
6	A:74:VAL:HG12	A:75:THR:HG23	0.625
6	A:26:VAL:HA	A:30:ALA:HB3	0.620
6	A:55:VAL:HG13	A:60:LYS:HB2	0.600
6	A:94:PHE:CE2	A:100:LEU:HD22	0.550
6	A:95:VAL:HG23	A:99:GLN:HB2	0.544
6	A:70:VAL:HG22	A:94:PHE:CE1	0.540
6	A:116:MET:HE1	A:133:TYR:CE1	0.507
6	A:90:ALA:HB3	A:120:PRO:HB3	0.488
6	A:46:GLU:HG2	A:74:VAL:HG11	0.487
6	A:96:LYS:HD2	A:98:ASP:HB2	0.438
6	A:62:GLN:HB3	A:62:GLN:HE21	0.432
6	A:19:ALA:HB3	A:24:GLN:HB2	0.429
6	A:136:TYR:CD2	A:140:ALA:HA	0.421
6	A:95:VAL:HG23	A:96:LYS:H	0.420
6	A:88:ILE:HA	A:88:ILE:HD12	0.410

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:119:ASP:HA	A:120:PRO:HD3	0.410
7	A:36:GLY:HA3	A:76:ALA:HB3	1.038
7	A:77:VAL:HG11	A:121:ASP:HB2	0.760
7	A:49:VAL:HG12	A:66:VAL:HA	0.717
7	A:35:GLU:HG2	A:48:VAL:HG11	0.605
7	A:55:VAL:HG21	A:102:LYS:HG2	0.603
7	A:107:ALA:HB3	A:116:MET:HB3	0.598
7	A:116:MET:SD	A:128:PRO:HG3	0.556
7	A:89:ALA:HB2	A:96:LYS:HB2	0.537
7	A:77:VAL:CG1	A:121:ASP:HB2	0.509
7	A:39:TYR:HD2	A:46:GLU:HB3	0.501
7	A:108:PRO:HA	A:114:GLU:HA	0.471
7	A:37:VAL:HG13	A:118:VAL:HG11	0.467
7	A:15:VAL:HG13	A:40:VAL:HB	0.465
7	A:54:THR:HG21	A:85:ALA:H	0.417
7	A:79:GLN:HB3	A:79:GLN:HE21	0.406
7	A:38:LEU:HD23	A:48:VAL:CG2	0.403
7	A:137:GLU:HB3	A:138:PRO:CD	0.402
8	A:10:LYS:HG3	A:18:ALA:HB3	0.761
8	A:99:GLN:HA	A:110:GLU:HB2	0.716
8	A:26:VAL:HB	A:113:LEU:HD13	0.676
8	A:56:ALA:HA	A:95:VAL:HG11	0.656
8	A:71:VAL:HG12	A:88:ILE:HD12	0.655

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:130:GLU:HB2	A:134:GLN:HE22	0.650
8	A:45:LYS:HA	A:48:VAL:HB	0.593
8	A:80:LYS:HB3	A:82:VAL:CG2	0.588
8	A:94:PHE:CZ	A:96:LYS:HB3	0.587
8	A:50:HIS:HB2	A:106:GLY:HA3	0.569
8	A:133:TYR:HB2	A:136:TYR:HB2	0.538
8	A:80:LYS:HB3	A:82:VAL:HG22	0.523
8	A:130:GLU:HB2	A:134:GLN:NE2	0.507
8	A:19:ALA:HB1	A:35:GLU:HG3	0.495
8	A:26:VAL:CG1	A:113:LEU:HD13	0.484
8	A:86:GLY:HA3	A:97:LYS:HD3	0.470
8	A:12:LYS:HB3	A:15:VAL:HG12	0.466
8	A:10:LYS:HG3	A:18:ALA:CB	0.455
8	A:26:VAL:CB	A:113:LEU:HD13	0.446
8	A:122:ASN:HA	A:122:ASN:HD22	0.428
8	A:20:GLU:HA	A:33:THR:HG22	0.424
8	A:59:THR:HB	A:95:VAL:HG12	0.418

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	138	81	27	30
2	138	90	24	24
3	138	83	22	33

Model ID	Analyzed	Favored	Allowed	Outliers
4	138	76	31	31
5	138	89	23	26
6	138	84	32	22
7	138	88	24	26
8	138	82	30	26

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	103	69	17	17
2	103	60	17	26
3	103	58	21	24
4	103	58	21	24
5	103	59	22	22
6	103	63	13	27
7	103	68	18	17
8	103	63	18	22

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	4	PHE
1	A	13	GLU
1	A	16	VAL
1	A	22	THR
1	A	39	TYR

Model ID	Chain	Residue ID	Residue type
1	A	55	VAL
1	A	71	VAL
1	A	80	LYS
1	A	88	ILE
1	A	92	THR
1	A	104	GLU
1	A	113	LEU
1	A	121	ASP
1	A	123	GLU
1	A	131	GLU
1	A	134	GLN
1	A	137	GLU
2	A	3	VAL
2	A	8	LEU
2	A	16	VAL
2	A	21	LYS
2	A	22	THR
2	A	40	VAL
2	A	48	VAL
2	A	52	VAL
2	A	54	THR
2	A	55	VAL
2	A	64	THR

Model ID	Chain	Residue ID	Residue type
2	A	66	VAL
2	A	71	VAL
2	A	72	THR
2	A	74	VAL
2	A	77	VAL
2	A	79	GLN
2	A	82	VAL
2	A	88	ILE
2	A	95	VAL
2	A	102	LYS
2	A	109	GLN
2	A	112	ILE
2	A	113	LEU
2	A	115	ASP
2	A	126	GLU
3	A	1	MET
3	A	2	ASP
3	A	4	PHE
3	A	8	LEU
3	A	12	LYS
3	A	13	GLU
3	A	16	VAL
3	A	20	GLU

Model ID	Chain	Residue ID	Residue type
3	A	32	LYS
3	A	52	VAL
3	A	59	THR
3	A	64	THR
3	A	66	VAL
3	A	70	VAL
3	A	71	VAL
3	A	72	THR
3	A	88	ILE
3	A	94	PHE
3	A	95	VAL
3	A	100	LEU
3	A	103	ASN
3	A	115	ASP
3	A	116	MET
3	A	118	VAL
4	A	13	GLU
4	A	16	VAL
4	A	21	LYS
4	A	34	LYS
4	A	38	LEU
4	A	39	TYR
4	A	40	VAL

Model ID	Chain	Residue ID	Residue type
4	A	44	THR
4	A	57	GLU
4	A	59	THR
4	A	62	GLN
4	A	63	VAL
4	A	66	VAL
4	A	77	VAL
4	A	88	ILE
4	A	94	PHE
4	A	110	GLU
4	A	112	ILE
4	A	115	ASP
4	A	116	MET
4	A	122	ASN
4	A	128	PRO
4	A	130	GLU
4	A	136	TYR
5	A	2	ASP
5	A	15	VAL
5	A	33	THR
5	A	38	LEU
5	A	48	VAL
5	A	54	THR

Model ID	Chain	Residue ID	Residue type
5	A	55	VAL
5	A	59	THR
5	A	64	THR
5	A	65	ASN
5	A	71	VAL
5	A	72	THR
5	A	81	THR
5	A	82	VAL
5	A	94	PHE
5	A	100	LEU
5	A	112	ILE
5	A	113	LEU
5	A	115	ASP
5	A	118	VAL
5	A	133	TYR
5	A	135	ASP
6	A	3	VAL
6	A	8	LEU
6	A	15	VAL
6	A	26	VAL
6	A	32	LYS
6	A	33	THR
6	A	38	LEU

Model ID	Chain	Residue ID	Residue type
6	A	43	LYS
6	A	44	THR
6	A	49	VAL
6	A	59	THR
6	A	62	GLN
6	A	64	THR
6	A	66	VAL
6	A	71	VAL
6	A	81	THR
6	A	82	VAL
6	A	83	GLU
6	A	88	ILE
6	A	98	ASP
6	A	100	LEU
6	A	109	GLN
6	A	113	LEU
6	A	114	GLU
6	A	125	TYR
6	A	126	GLU
6	A	134	GLN
7	A	1	MET
7	A	8	LEU
7	A	9	SER

Model ID	Chain	Residue ID	Residue type
7	A	12	LYS
7	A	26	VAL
7	A	38	LEU
7	A	49	VAL
7	A	62	GLN
7	A	74	VAL
7	A	79	GLN
7	A	88	ILE
7	A	92	THR
7	A	98	ASP
7	A	105	GLU
7	A	112	ILE
7	A	115	ASP
7	A	131	GLU
8	A	2	ASP
8	A	3	VAL
8	A	4	PHE
8	A	26	VAL
8	A	32	LYS
8	A	52	VAL
8	A	54	THR
8	A	55	VAL
8	A	59	THR

Model ID	Chain	Residue ID	Residue type
8	A	60	LYS
8	A	64	THR
8	A	66	VAL
8	A	74	VAL
8	A	81	THR
8	A	82	VAL
8	A	92	THR
8	A	99	GLN
8	A	100	LEU
8	A	121	ASP
8	A	122	ASN
8	A	133	TYR
8	A	139	GLU

Fit of model to data used for modeling

Fit of model to data used for validation

Validation for this section is under development.

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