Integrative Structure Validation Report

July 22, 2024 - 04:33 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	9A1H
PDB-Dev ID	PDBDEV_00000089
Structure Title	Integrative structural model of alpha-synuclein compact states bound to membrane mimics
Structure Authors	Schwarz, Thomas C.; Beier, Andreas; Ledolter, Karin; Gossenreiter, Thomas; Hofurthner, Theresa; Hartl, Markus; Baker, Terry S.; Taylor, Richard J.; Konrat, Robert

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

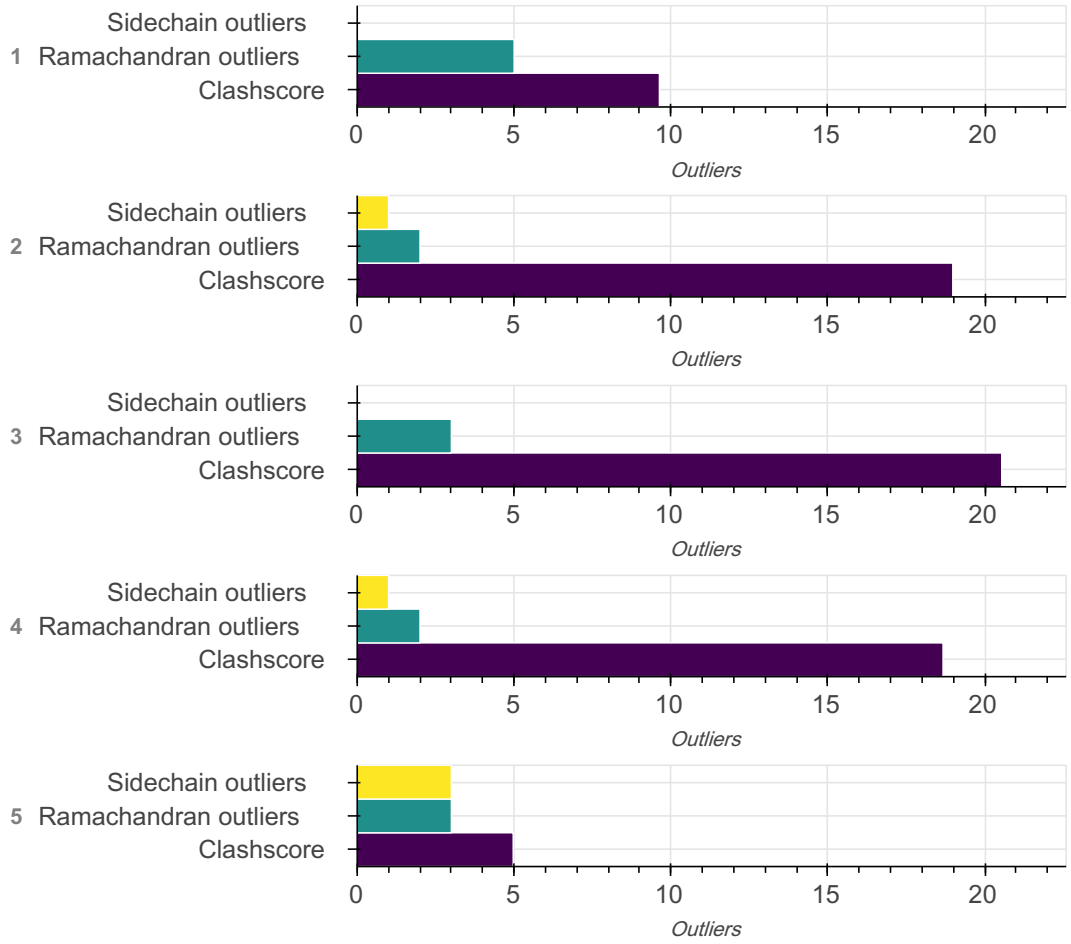
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 5 unique models, with 2 subunits in each model. A total of 2 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 5 unique types of models in this entry.These models are titled None, None, None, None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	alpha-synuclein	A	A	110
1	2	1	alpha-synuclein	B	B	110
2	1	1	alpha-synuclein	A	A	110
2	2	1	alpha-synuclein	B	B	110
3	1	1	alpha-synuclein	A	A	110
3	2	1	alpha-synuclein	B	B	110
4	1	1	alpha-synuclein	A	A	110
4	2	1	alpha-synuclein	B	B	110
5	1	1	alpha-synuclein	A	A	110
5	2	1	alpha-synuclein	B	B	110

Datasets used for modeling

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD027349
2	NMR data	BMRB	50996

Representation

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

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-110
B	-	1-110

Methodology and software

This entry is a result of 2 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	Simulated Annealing	Simulated annealing of the monomer	None	2700	False	False
1	2	Simulated Annealing	Simulated annealing of the dimer	None	1500	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	XPLOR-NIH	1.49	structure determination program	https://nmr.cit.nih.gov/xplor-nih/

Data quality

NMR

Validation for this section is under development.

Crosslinking-MS

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 5593 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
CA--HA	1.07	0.97	1
CA--HA	1.08	0.97	657
CA--HA1	1.08	0.97	112
CA--HA2	1.08	0.97	112
OH--HH	0.96	0.84	7
OG1--HG1	0.96	0.84	53
OG--HG	0.96	0.84	10
OG1--HG1	0.97	0.84	10
OG--HG	0.97	0.84	4
N--HN	0.99	0.86	49
CB--HB1	1.10	0.97	1
CG1--HG13	1.10	0.97	1
N--HN	1.00	0.86	697
CG2--HG23	1.11	0.97	196
CB--HB1	1.11	0.97	461
NE2--HE22	1.00	0.86	35
CG1--HG11	1.11	0.97	133
ND2--HD22	1.00	0.86	14
CG1--HG12	1.11	0.97	133

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--HD21	1.00	0.86	14
CG--HG1	1.11	0.97	231
NE2--HE21	1.00	0.86	35
CG--HG2	1.11	0.97	231
CB--HB2	1.11	0.97	462
CG2--HG22	1.11	0.97	196
CB--HB	1.11	0.97	196
CG1--HG13	1.11	0.97	125
CG--HG	1.11	0.97	21
CG2--HG21	1.11	0.97	196
CE--HE2	1.11	0.97	119
CB--HB3	1.11	0.97	112
CD1--HD13	1.11	0.97	28
CD--HD2	1.11	0.97	112
CE--HE1	1.11	0.97	119
NE2--HE2	1.00	0.86	7
CE--HE3	1.11	0.97	14
CD1--HD11	1.11	0.97	28
CD2--HD23	1.11	0.97	21
CD1--HD12	1.11	0.97	28
CD--HD1	1.11	0.97	112
CD2--HD21	1.11	0.97	21
CD2--HD22	1.11	0.97	21

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N--HN	1.01	0.86	9
CD1--HD1	1.08	0.93	21
CE2--HE2	1.08	0.93	21
NZ--HZ3	1.04	0.89	104
NZ--HZ2	1.04	0.89	105
CD2--HD2	1.08	0.93	28
NZ--HZ1	1.04	0.89	104
CE1--HE1	1.08	0.93	21
N--HT2	1.04	0.89	7
N--HT3	1.04	0.89	7
N--HT1	1.04	0.89	7
CZ--HZ	1.08	0.93	14
NZ--HZ3	1.05	0.89	1
NZ--HZ1	1.05	0.89	1
CE1--HE1	1.09	0.93	7
N--HN	1.02	0.86	1

Standard geometry: angle outliers

There are 7 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
ND1-CG-CD2	106.10	110.47	1
ND1-CG-CD2	106.10	110.46	2
ND1-CG-CD2	106.10	110.45	2
ND1-CG-CD2	106.10	110.39	2

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	9.63	31
2	18.98	61
3	20.54	33
4	18.67	30
5	4.97	8

All 163 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	B:104:CYS:O	B:104:CYS:SG1	1.137
1	A:104:CYS:O	A:104:CYS:SG1	1.132
1	A:19:CYS:SG1	A:23:LYS:HE3	0.777
1	B:19:CYS:SG1	B:23:LYS:HE3	0.777
1	A:16:VAL:HG12	A:19:CYS:CB	0.690
1	B:16:VAL:HG12	B:19:CYS:CB	0.686
1	B:19:CYS:CL1	B:23:LYS:CE	0.640
1	B:104:CYS:CS8	B:104:CYS:SG2	0.636
1	A:104:CYS:CS8	A:104:CYS:SG2	0.635
1	A:19:CYS:CL1	A:23:LYS:CE	0.617
1	B:19:CYS:CL1	B:23:LYS:HE2	0.609
1	A:19:CYS:CL1	A:23:LYS:HE2	0.598
1	A:40:VAL:HG12	A:43:LYS:HB2	0.558
1	B:16:VAL:CG1	B:19:CYS:CB	0.557
1	A:16:VAL:CG1	A:19:CYS:CB	0.554

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:42:CYS:O	B:42:CYS:SG1	0.554
1	B:40:VAL:HG12	B:43:LYS:HB2	0.550
1	B:19:CYS:CL1	B:23:LYS:HE3	0.546
1	A:42:CYS:O	A:42:CYS:SG1	0.544
1	A:19:CYS:CL1	A:23:LYS:HE3	0.534
1	A:78:ALA:O	A:82:VAL:HG23	0.508
1	B:78:ALA:O	B:82:VAL:HG23	0.506
1	A:88:ILE:O	A:88:ILE:HG22	0.472
1	B:88:ILE:O	B:88:ILE:HG22	0.472
1	B:73:GLY:O	B:77:VAL:HG23	0.445
1	A:73:GLY:O	A:77:VAL:HG23	0.434
1	B:70:VAL:O	B:74:VAL:HG23	0.432
1	B:16:VAL:HG12	B:19:CYS:H	0.407
1	B:22:THR:O	B:26:VAL:HG23	0.407
1	A:70:VAL:O	A:74:VAL:HG23	0.406
1	B:39:TYR:C	B:40:VAL:HG23	0.403
2	A:19:CYS:CS7	B:52:VAL:HG13	1.365
2	A:81:CYS:CS8	B:65:ASN:HA	1.286
2	A:104:CYS:CS9	A:104:CYS:SG1	1.240
2	A:81:CYS:CS8	B:65:ASN:CA	1.239
2	B:104:CYS:CS9	B:104:CYS:SG1	1.238
2	A:19:CYS:CS7	B:52:VAL:CG1	1.237
2	A:88:ILE:HD12	B:104:CYS:CS5	1.141

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:19:CYS:O	B:19:CYS:SG1	1.089
2	A:88:ILE:HD12	B:104:CYS:CS6	1.082
2	A:81:CYS:CS9	B:65:ASN:CA	1.061
2	A:88:ILE:HD12	B:104:CYS:CS4	1.040
2	A:19:CYS:O	A:19:CYS:SG1	1.016
2	A:81:CYS:CS9	B:65:ASN:O	0.976
2	A:88:ILE:CD1	B:104:CYS:CS7	0.971
2	B:19:CYS:O	B:19:CYS:SG2	0.971
2	B:19:CYS:C	B:19:CYS:SG2	0.943
2	B:16:VAL:O	B:19:CYS:SG2	0.938
2	A:16:VAL:O	A:19:CYS:SG2	0.928
2	A:88:ILE:CD1	B:104:CYS:CS6	0.925
2	A:81:CYS:CS9	B:65:ASN:HA	0.894
2	A:19:CYS:C	A:19:CYS:SG2	0.877
2	A:81:CYS:CS9	B:65:ASN:C	0.825
2	A:88:ILE:CD1	B:104:CYS:CS5	0.824
2	A:19:CYS:O	A:19:CYS:SG2	0.811
2	A:19:CYS:OS1	B:55:VAL:HG11	0.774
2	A:42:CYS:CL1	A:46:GLU:OE2	0.758
2	B:42:CYS:CL1	B:46:GLU:OE2	0.750
2	A:19:CYS:OS1	B:55:VAL:CG1	0.731
2	A:88:ILE:HD12	B:104:CYS:CS7	0.723
2	B:101:GLY:O	B:104:CYS:CS8	0.694

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:19:CYS:CS7	B:52:VAL:HG12	0.686
2	A:88:ILE:HD13	B:104:CYS:CS7	0.684
2	A:101:GLY:O	A:104:CYS:CS8	0.671
2	A:70:VAL:O	A:74:VAL:HG23	0.612
2	A:88:ILE:HD11	B:104:CYS:CS6	0.603
2	B:70:VAL:O	B:74:VAL:HG23	0.598
2	B:19:CYS:CS6	B:23:LYS:O	0.597
2	A:81:CYS:CS8	B:65:ASN:N	0.595
2	A:19:CYS:CS6	A:23:LYS:O	0.589
2	B:42:CYS:CS3	B:46:GLU:OE2	0.551
2	A:104:CYS:CS8	A:104:CYS:SG2	0.542
2	B:78:ALA:O	B:82:VAL:HG23	0.538
2	A:42:CYS:CS3	A:46:GLU:OE2	0.536
2	B:104:CYS:CS8	B:104:CYS:SG2	0.532
2	A:19:CYS:CS6	B:52:VAL:HG13	0.530
2	A:78:ALA:O	A:82:VAL:HG23	0.530
2	A:88:ILE:CD1	B:104:CYS:CS4	0.516
2	A:18:ALA:C	A:20:GLU:H	0.471
2	B:39:TYR:C	B:40:VAL:HG23	0.470
2	A:19:CYS:CS5	B:52:VAL:HG13	0.465
2	B:18:ALA:C	B:20:GLU:H	0.453
2	A:19:CYS:SG1	A:23:LYS:HG2	0.431
2	B:64:THR:O	B:64:THR:HG22	0.426

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:39:TYR:C	A:40:VAL:HG23	0.424
2	A:64:THR:O	A:64:THR:HG22	0.412
2	B:19:CYS:SG1	B:22:THR:HB	0.408
2	A:19:CYS:SG1	A:22:THR:HB	0.405
2	B:19:CYS:SG1	B:23:LYS:HG2	0.405
2	B:42:CYS:O	B:42:CYS:SG1	0.402
2	A:22:THR:O	A:26:VAL:HG23	0.400
2	A:51:GLY:O	A:55:VAL:HG23	0.400
3	A:19:CYS:CS3	A:23:LYS:CB	1.225
3	A:104:CYS:CS8	A:106:GLY:HA2	1.194
3	A:19:CYS:CS6	A:21:LYS:HA	1.171
3	A:19:CYS:CL1	A:23:LYS:HB2	1.162
3	A:19:CYS:CS7	A:24:GLN:HG3	1.159
3	A:104:CYS:CS8	A:106:GLY:CA	1.134
3	A:19:CYS:CS4	A:23:LYS:HB3	1.120
3	A:19:CYS:CS6	A:21:LYS:CA	1.008
3	A:19:CYS:CS4	A:23:LYS:CB	0.946
3	A:19:CYS:CS3	A:23:LYS:HB2	0.866
3	A:104:CYS:SG1	A:105:GLU:O	0.864
3	A:19:CYS:NS1	A:24:GLN:N	0.777
3	A:19:CYS:CL1	A:23:LYS:CB	0.768
3	A:103:ASN:HB2	A:104:CYS:CS6	0.755
3	A:103:ASN:CB	A:104:CYS:CS6	0.751

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:103:ASN:O	A:104:CYS:CB	0.749
3	A:71:VAL:O	A:74:VAL:HG22	0.690
3	A:19:CYS:CS6	A:21:LYS:N	0.597
3	A:103:ASN:HB3	A:104:CYS:CS6	0.594
3	A:19:CYS:NS1	A:21:LYS:CA	0.550
3	A:19:CYS:OS1	A:24:GLN:HB2	0.549
3	A:19:CYS:CL1	A:23:LYS:CA	0.548
3	A:19:CYS:OS1	A:24:GLN:N	0.543
3	A:42:CYS:CS8	A:45:LYS:HE2	0.530
3	A:19:CYS:CS7	A:23:LYS:HB3	0.522
3	A:19:CYS:CS6	A:20:GLU:HG2	0.513
3	A:19:CYS:CS5	A:23:LYS:HB3	0.504
3	A:103:ASN:HB3	A:104:CYS:CS7	0.447
3	A:22:THR:O	A:26:VAL:HG23	0.432
3	A:39:TYR:C	A:41:GLY:H	0.420
3	A:40:VAL:O	A:40:VAL:HG12	0.414
3	A:19:CYS:CS5	A:21:LYS:CA	0.411
3	A:19:CYS:CS7	A:24:GLN:N	0.401
4	A:95:VAL:HG13	A:104:CYS:CS7	1.228
4	A:42:CYS:CL1	A:45:LYS:HZ3	1.209
4	A:99:GLN:HA	A:104:CYS:SG2	1.196
4	A:42:CYS:CS3	A:45:LYS:HZ3	0.973
4	A:42:CYS:CS3	A:45:LYS:NZ	0.887

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:42:CYS:CL1	A:45:LYS:NZ	0.871
4	A:99:GLN:CA	A:104:CYS:SG2	0.844
4	A:95:VAL:CG1	A:104:CYS:CS7	0.797
4	A:42:CYS:CS9	A:45:LYS:NZ	0.696
4	A:96:LYS:H	A:104:CYS:CS6	0.674
4	A:98:ASP:O	A:104:CYS:SG1	0.662
4	A:96:LYS:N	A:104:CYS:CS6	0.656
4	A:33:THR:HG22	A:38:LEU:HB2	0.642
4	A:42:CYS:CS9	A:45:LYS:HZ2	0.612
4	A:101:GLY:N	A:104:CYS:CS8	0.606
4	A:90:ALA:HB1	A:96:LYS:HB2	0.603
4	A:48:VAL:O	A:52:VAL:HG23	0.515
4	A:59:THR:O	A:63:VAL:HG23	0.501
4	A:42:CYS:CS3	A:45:LYS:HZ2	0.475
4	A:45:LYS:O	A:49:VAL:HG23	0.470
4	A:81:CYS:O	A:81:CYS:SG1	0.464
4	A:98:ASP:O	A:104:CYS:CS8	0.457
4	A:71:VAL:HG22	A:103:ASN:HD21	0.439
4	A:4:PHE:CZ	A:5:MET:HE2	0.438
4	A:70:VAL:O	A:74:VAL:HG22	0.423
4	A:51:GLY:O	A:55:VAL:HG23	0.419
4	A:34:LYS:HA	A:38:LEU:HB3	0.406
4	A:22:THR:O	A:26:VAL:HG23	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:99:GLN:N	A:104:CYS:CS6	0.402
4	A:104:CYS:CS8	A:104:CYS:SG1	0.401
5	A:103:ASN:O	A:104:CYS:CB	0.778
5	A:38:LEU:O	A:42:CYS:CB	0.569
5	A:70:VAL:O	A:74:VAL:HG23	0.555
5	A:73:GLY:O	A:77:VAL:HG23	0.496
5	A:37:VAL:HG23	A:52:VAL:HG22	0.479
5	A:48:VAL:O	A:52:VAL:HG23	0.459
5	A:11:ALA:O	A:15:VAL:HG23	0.419
5	A:95:VAL:HG13	A:96:LYS:N	0.413

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	152	141	6	5
2	151	140	9	2
3	151	145	3	3
4	151	141	8	2
5	151	132	16	3

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	104	101	3	0

Model ID	Analyzed	Favored	Allowed	Outliers
2	104	102	1	1
3	103	102	1	0
4	104	103	0	1
5	103	96	4	3

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
2	A	40	VAL
4	A	63	VAL
5	A	87	SER
5	A	100	LEU
5	A	22	THR

Fit of model to data used for modeling

NMR

Validation for this section is under development.

Crosslinking-MS

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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