

Integrative Structure Validation Report ?

April 03, 2025 - 08:38 AM PDT

The following software was used in the production of this report:

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	9A2E
PDB-Dev ID	PDBDEV_00000161
Structure Title	Structures of the PSG Supramodule of PSD-95 Resolved by Integrative FRET
Structure Authors	Hamilton, G.; Saikia, N.; Basak, S.; Welcome, F. S.; Wu, F.; Kubiak, J.; Zhang, C.; Hao, Y.; Seidel, C. A. M.; Ding, F.; Sanabria, H.; Bowen, M. E.
Deposited on	2022-09-08

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

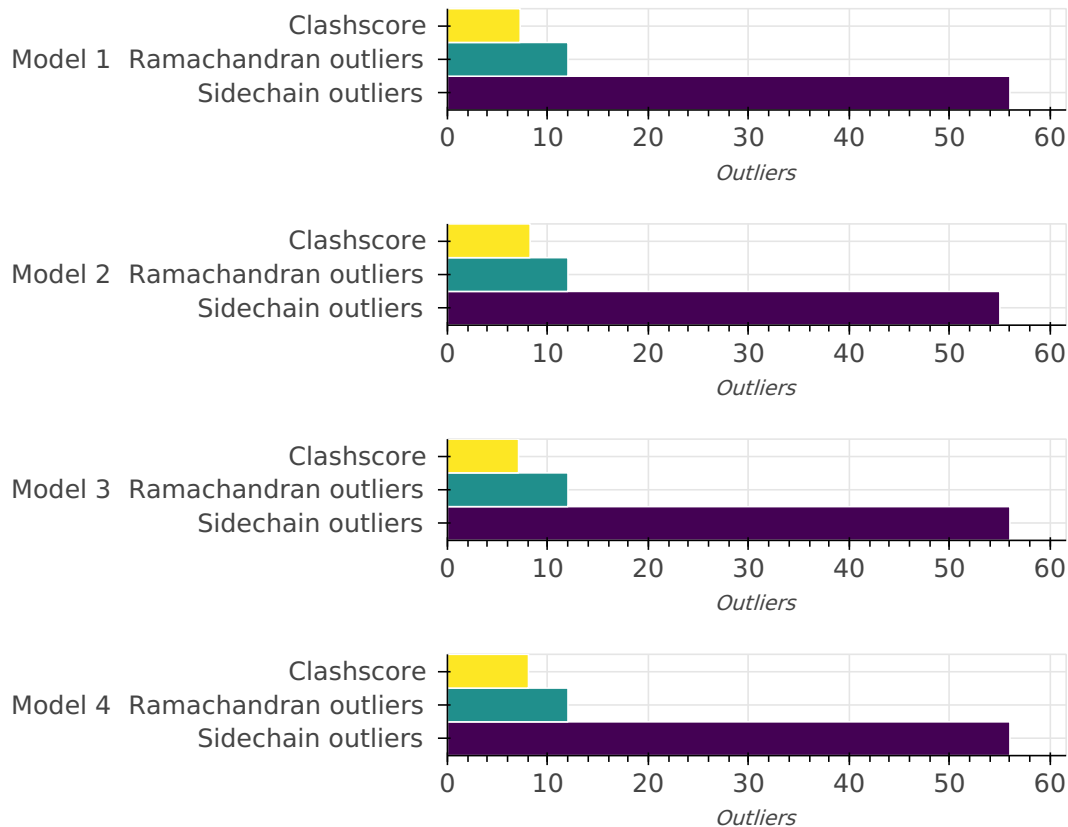
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 and fit to model assessments for SAS and crosslinking-MS 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 model(s). A total of 36 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1-4	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	724	313-724	-	56.91 / 100.00	Atomic

Datasets used for modeling ?

There are 36 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
2	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
3	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
4	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
5	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
6	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
7	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
8	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
9	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
10	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
11	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
12	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
13	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
14	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
15	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
16	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
17	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
18	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
19	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
20	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
21	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
22	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978

ID	Dataset type	Database name	Data access code
23	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
24	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
25	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
26	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
27	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
28	Predicted contacts	Zenodo	10.5281/zenodo.7125978
29	Predicted contacts	Zenodo	10.5281/zenodo.7125978
30	Predicted contacts	Zenodo	10.5281/zenodo.7125978
31	Predicted contacts	Zenodo	10.5281/zenodo.7125978
32	Comparative model	Zenodo	10.5281/zenodo.7125978
34	Experimental model	Zenodo	10.5281/zenodo.7125978
35	Experimental model	Zenodo	10.5281/zenodo.7125978
33	Integrative model	Not available	Not available
36	Other	Not available	Not available

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	FRET-guided rigid body docking	None	None	None	True	False
1	2	FRET-guided rigid body docking with disulfide mapping restraints	None	None	None	True	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	FRET Positioning and Screening (FPS)	1.10	Model Building	https://www.mpc.hhu.de/en/software/fps

Data quality ?

Predicted contacts

Validation for this section is under development.

Single molecule FRET

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 no bond length outliers.

Standard geometry: angle outliers ?

There are 122 bond angle outliers in this entry (0.72% of 16900 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	581	HIS	CB-CG-CD2	7.71	121.18	131.20	4	4
A	550	ASP	CA-CB-CG	6.81	119.41	112.60	4	4
A	664	ARG	CD-NE-CZ	6.70	133.78	124.40	4	4
A	539	ILE	C-N-CA	6.64	133.66	121.70	2	4
A	586	ARG	CD-NE-CZ	5.97	132.76	124.40	2	4
A	581	HIS	CA-CB-CG	5.77	108.03	113.80	1	4
A	565	HIS	C-CA-CB	5.47	120.50	110.10	1	4
A	565	HIS	C-N-CA	5.46	131.52	121.70	3	4
A	565	HIS	CB-CG-CD2	5.40	124.18	131.20	2	4
A	539	ILE	C-CA-CB	5.24	122.07	111.60	2	4
A	702	HIS	CB-CG-CD2	5.20	124.44	131.20	1	4
A	565	HIS	CA-CB-CG	5.04	108.76	113.80	1	4
A	605	ASN	C-N-CA	5.00	130.69	121.70	4	4
A	596	HIS	CB-CG-CD2	4.86	124.88	131.20	4	4
A	664	ARG	NE-CZ-NH1	4.63	126.13	121.50	2	4
A	348	ASP	CA-CB-CG	4.53	117.13	112.60	3	4
A	669	GLN	OE1-CD-NE2	4.52	118.08	122.60	1	4
A	593	ILE	CA-CB-CG1	4.40	117.88	110.40	1	4
A	642	HIS	CB-CG-CD2	4.36	125.53	131.20	2	4
A	688	PHE	CA-CB-CG	4.31	118.11	113.80	2	4
A	489	PRO	N-CA-CB	4.30	107.73	103.00	4	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	548	ASN	OD1-CG-ND2	4.25	118.35	122.60	3	4
A	596	HIS	CA-CB-CG	4.21	118.01	113.80	4	4
A	639	GLN	OE1-CD-NE2	4.20	118.40	122.60	1	4
A	690	ALA	C-N-CA	4.17	129.21	121.70	4	4
A	644	HIS	CB-CG-CD2	4.16	125.79	131.20	2	4
A	724	LEU	CD1-CG-CD2	4.13	101.72	110.80	1	4
A	594	GLN	OE1-CD-NE2	4.11	118.49	122.60	1	4
A	578	ARG	CD-NE-CZ	4.08	130.11	124.40	3	3
A	625	HIS	CB-CG-CD2	4.06	125.92	131.20	1	4
A	452	LEU	CD1-CG-CD2	4.02	101.95	110.80	3	2
A	381	ASN	CA-CB-CG	4.01	116.61	112.60	3	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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	7.25	44
2	8.23	50
3	7.08	43
4	8.07	49

There are 186 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:349:LEU:HD21	A:633:ASN:OD1	1.04	4	1
A:473:ALA:HB2	A:488:ILE:HB	1.03	2	4
A:351:GLY:HA3	A:500:SER:OG	0.87	2	1
A:431:PHE:HB3	A:462:VAL:HB	0.85	4	4
A:448:LEU:HD13	A:451:ALA:HB3	0.79	4	4
A:338:ILE:HD11	A:359:ILE:HD11	0.75	2	4
A:360:LEU:HB2	A:389:ILE:HG22	0.74	2	4
A:473:ALA:CB	A:488:ILE:HB	0.71	2	4
A:473:ALA:HB2	A:488:ILE:CB	0.68	2	4
A:452:LEU:HD21	A:475:ARG:HB2	0.67	4	4

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:337:PHE:CE2	A:358:GLN:HG2	0.66	3	4
A:525:THR:HG23	A:724:LEU:HD22	0.64	4	4
A:539:ILE:HG22	A:540:LEU:H	0.63	4	4
A:336:ILE:HG21	A:375:ALA:HB2	0.63	1	4
A:431:PHE:HD2	A:462:VAL:HG11	0.62	4	4
A:349:LEU:HD21	A:633:ASN:CG	0.59	4	1
A:475:ARG:HE	A:482:THR:HG21	0.57	3	4
A:354:ARG:HE	A:503:LYS:HG2	0.57	2	1
A:428:LYS:HB2	A:721:ARG:HH22	0.56	4	4
A:360:LEU:HB2	A:389:ILE:CG2	0.56	1	4
A:431:PHE:CD2	A:462:VAL:HG11	0.55	4	4
A:463:ILE:HB	A:472:GLN:HB3	0.54	4	4
A:395:GLU:O	A:396:GLU:C	0.53	2	4
A:525:THR:CG2	A:724:LEU:HD22	0.49	4	4
A:491:LYS:H	A:491:LYS:HG3	0.49	4	2
A:526:VAL:HB	A:717:TRP:CB	0.49	3	4
A:329:GLY:HA2	A:336:ILE:HG22	0.48	1	4
A:526:VAL:HB	A:717:TRP:HB3	0.48	3	4
A:354:ARG:NE	A:503:LYS:HG2	0.48	2	1
A:336:ILE:HG13	A:359:ILE:HB	0.47	3	4
A:452:LEU:HB2	A:486:GLY:HA3	0.47	2	4
A:656:GLU:CD	A:656:GLU:H	0.47	3	4
A:316:ILE:HD12	A:325:PHE:HE1	0.46	2	4
A:436:LEU:HD22	A:686:GLU:HA	0.46	1	4
A:343:ALA:HB2	A:505:LYS:HE2	0.45	2	1
A:439:TYR:HE1	A:448:LEU:HD11	0.45	4	4
A:452:LEU:HD21	A:475:ARG:CB	0.45	4	4
A:433:ILE:HG22	A:460:LEU:HB2	0.45	1	4
A:502:LEU:HA	A:502:LEU:HD12	0.45	1	4
A:349:LEU:O	A:350:SER:C	0.44	2	4
A:459:VAL:HG11	A:717:TRP:CD1	0.44	4	4
A:435:ALA:HB2	A:454:PHE:HE2	0.43	3	4
A:338:ILE:HD11	A:359:ILE:CD1	0.43	4	2
A:431:PHE:HA	A:431:PHE:HD1	0.43	3	4
A:436:LEU:HA	A:456:PHE:CE1	0.42	3	4

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:475:ARG:NE	A:482:THR:HG21	0.42	3	4
A:349:LEU:CD2	A:633:ASN:OD1	0.42	4	1
A:455:ARG:H	A:455:ARG:HG2	0.41	3	4
A:464:ASP:HB3	A:465:ALA:H	0.41	1	4
A:719:PRO:HB3	A:720:ALA:H	0.41	4	4
A:325:PHE:HD1	A:347:ALA:HB2	0.41	2	2
A:431:PHE:HB3	A:462:VAL:CB	0.40	4	4
A:443:LYS:HD2	A:452:LEU:HA	0.40	4	4
A:393:LYS:HA	A:394:PRO:HD3	0.40	4	1

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	Analysed	Favored	Allowed	Outliers
1	379	334	33	12
2	379	335	32	12
3	379	334	33	12
4	379	335	32	12

There are 12 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	363	ASN	4
A	392	TYR	4
A	442	THR	4
A	468	GLU	4
A	514	GLN	4
A	515	GLY	4
A	539	ILE	4
A	540	LEU	4
A	565	HIS	4
A	566	THR	4
A	663	LYS	4
A	719	PRO	4

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	327	225	46	56
2	327	225	47	55
3	327	225	46	56
4	327	225	46	56

There are 56 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	316	ILE	4
A	318	ARG	4
A	323	LEU	4
A	327	ILE	4
A	334	GLU	4
A	346	PRO	4
A	350	SER	4
A	369	ASN	4
A	371	SER	4
A	374	GLN	4
A	384	GLN	4
A	386	VAL	4
A	387	THR	4
A	389	ILE	4
A	431	PHE	4
A	437	PHE	4
A	438	ASP	4
A	445	CYS	4
A	449	SER	4
A	458	ASP	4
A	459	VAL	4
A	464	ASP	4
A	470	TRP	4
A	474	ARG	4
A	481	GLU	4
A	482	THR	4
A	491	LYS	4
A	494	VAL	4

Chain	Res	Type	Models (Total)
A	497	ARG	4
A	502	LEU	4
A	514	GLN	4
A	520	VAL	4
A	521	LEU	4
A	525	THR	4
A	526	VAL	4
A	527	THR	4
A	544	LYS	4
A	545	ASP	4
A	567	THR	4
A	590	GLU	4
A	596	HIS	4
A	605	ASN	4
A	617	ARG	4
A	618	GLU	4
A	624	LYS	4
A	629	ASP	4
A	671	ARG	4
A	679	LYS	4
A	685	THR	4
A	686	GLU	4
A	687	CYS	4
A	716	ILE	4
A	718	VAL	4
A	721	ARG	4
A	723	ARG	4
A	483	ASP	3

Fit of model to data used for modeling ?

Predicted contacts

Validation for this section is under development.

Single molecule FRET

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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