Integrative Structure Validation Report

July 22, 2024 - 04:54 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	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.

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

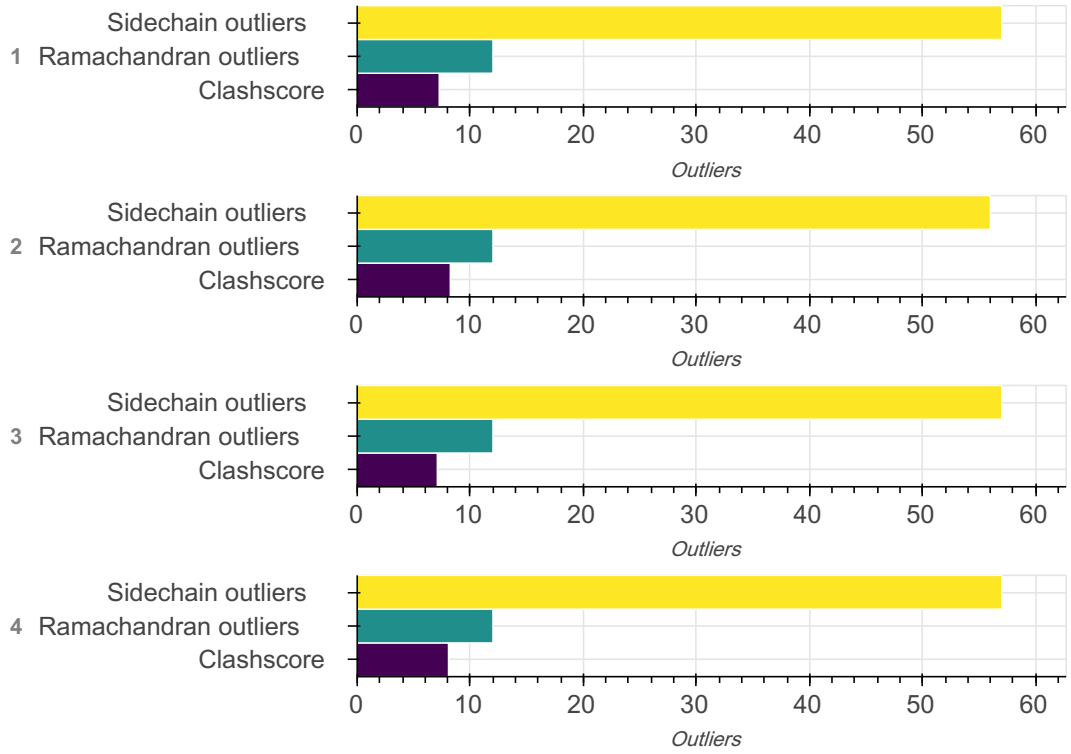
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 3 subunits in each model. A total of 36 datasets or restraints were used to build this entry. Each model is represented by 1 rigid bodies and 0 flexible or non-rigid units.

Entry composition

There are 4 unique types of models in this entry.These models are titled A, A, B, B respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	412
1	2	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	86

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	3	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	297
2	1	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	412
2	2	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	86
2	3	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	297
3	1	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	412
3	2	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	86
3	3	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	297
4	1	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	412
4	2	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	86
4	3	3	Postsynaptic density protein 95 (PSD95) Wild-Type	A	A	297

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	File	10.5281/zenodo.7125978
2	Single molecule FRET data	File	10.5281/zenodo.7125978
3	Single molecule FRET data	File	10.5281/zenodo.7125978
4	Single molecule FRET data	File	10.5281/zenodo.7125978

ID	Dataset type	Database name	Data access code
5	Single molecule FRET data	File	10.5281/zenodo.7125978
6	Single molecule FRET data	File	10.5281/zenodo.7125978
7	Single molecule FRET data	File	10.5281/zenodo.7125978
8	Single molecule FRET data	File	10.5281/zenodo.7125978
9	Single molecule FRET data	File	10.5281/zenodo.7125978
10	Single molecule FRET data	File	10.5281/zenodo.7125978
11	Single molecule FRET data	File	10.5281/zenodo.7125978
12	Single molecule FRET data	File	10.5281/zenodo.7125978
13	Single molecule FRET data	File	10.5281/zenodo.7125978
14	Single molecule FRET data	File	10.5281/zenodo.7125978
15	Single molecule FRET data	File	10.5281/zenodo.7125978
16	Single molecule FRET data	File	10.5281/zenodo.7125978
17	Single molecule FRET data	File	10.5281/zenodo.7125978
18	Single molecule FRET data	File	10.5281/zenodo.7125978
19	Single molecule FRET data	File	10.5281/zenodo.7125978
20	Single molecule FRET data	File	10.5281/zenodo.7125978
21	Single molecule FRET data	File	10.5281/zenodo.7125978
22	Single molecule FRET data	File	10.5281/zenodo.7125978
23	Single molecule FRET data	File	10.5281/zenodo.7125978
24	Single molecule FRET data	File	10.5281/zenodo.7125978
25	Single molecule FRET data	File	10.5281/zenodo.7125978
26	Single molecule FRET data	File	10.5281/zenodo.7125978
27	Single molecule FRET data	File	10.5281/zenodo.7125978

ID	Dataset type	Database name	Data access code
28	Other	File	10.5281/zenodo.7125978
29	Other	File	10.5281/zenodo.7125978
30	Other	File	10.5281/zenodo.7125978
31	Other	File	10.5281/zenodo.7125978
32	Comparative model	File	10.5281/zenodo.7125978
34	Experimental model	PDB	1KJW
35	Experimental model	PDB	6QJD
33	Integrative model	Not available	Not available
36	Other	Not available	Not available

Representation

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

Chain ID	Rigid bodies	Non-rigid segments
A	313-724	-

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	None	FRET-guided rigid body docking	None	None	True	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	2	None	FRET-guided rigid body docking with disulfide mapping restraints	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)	1.100	Model Building	https://www.mpc.hhu.de/en/software/fps

Data quality

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 2880 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
NZ--HZ3	0.98	0.89	4
NZ--HZ2	0.98	0.89	10
NZ--HZ2	0.99	0.89	15
NZ--HZ3	0.99	0.89	27
NZ--HZ1	0.99	0.89	27
NZ--HZ1	1.00	0.89	37

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ2	1.00	0.89	51
NZ--HZ3	1.00	0.89	46
N--H	0.97	0.86	4
SG--HG	1.31	1.20	1
NZ--HZ3	1.01	0.89	7
SG--HG	1.32	1.20	3
NZ--HZ1	1.01	0.89	11
N--H	0.98	0.86	74
NZ--HZ2	1.01	0.89	8
NH2--HH21	0.98	0.86	4
NE2--HE21	0.98	0.86	4
NH2--HH22	0.98	0.86	4
NH1--HH12	0.98	0.86	4
N--H	0.99	0.86	202
NZ--HZ1	1.02	0.89	9
NE2--HE22	0.99	0.86	16
ND2--HD22	0.99	0.86	8
ND2--HD21	0.99	0.86	4
NE2--HE21	0.99	0.86	8
NH1--HH12	0.99	0.86	10
NH2--HH22	0.99	0.86	8
NE--HE	0.99	0.86	8
NH1--HH11	0.99	0.86	4

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
SG--HG	1.33	1.20	3
NH2--HH21	0.99	0.86	3
N--H	1.00	0.86	801
SG--HG	1.34	1.20	9
NH2--HH21	1.00	0.86	74
NE--HE	1.00	0.86	61
NE2--HE21	1.00	0.86	39
NH1--HH12	1.00	0.86	58
NE1--HE1	1.00	0.86	4
ND1--HD1	1.00	0.86	40
ND2--HD22	1.00	0.86	16
NE2--HE22	1.00	0.86	28
ND2--HD21	1.00	0.86	20
NH2--HH22	1.00	0.86	71
NH1--HH11	1.00	0.86	68
OG--HG	0.98	0.84	16
OG1--HG1	0.98	0.84	4
OH--HH	0.98	0.84	4
N--H	1.01	0.86	295
NH2--HH22	1.01	0.86	20
NE2--HE21	1.01	0.86	5
NH2--HH21	1.01	0.86	27
NH1--HH11	1.01	0.86	42

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG--HG	0.99	0.84	24
ND2--HD21	1.01	0.86	4
ND1--HD1	1.01	0.86	12
NE--HE	1.01	0.86	30
OG1--HG1	0.99	0.84	9
OH--HH	0.99	0.84	14
ND2--HD22	1.01	0.86	10
NE2--HE22	1.01	0.86	4
NH1--HH12	1.01	0.86	35
NE1--HE1	1.01	0.86	9
NH1--HH12	1.02	0.86	21
NE--HE	1.02	0.86	29
N--H	1.02	0.86	104
NH2--HH22	1.02	0.86	25
NH1--HH11	1.02	0.86	14
ND2--HD22	1.02	0.86	2
NH2--HH21	1.02	0.86	20
ND2--HD21	1.02	0.86	8
NE1--HE1	1.02	0.86	7
OG--HG	1.00	0.84	60
NE2--HE21	1.02	0.86	4
OH--HH	1.00	0.84	26
OG1--HG1	1.00	0.84	29

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE22	1.02	0.86	12
OG1--HG1	1.01	0.84	14
OH--HH	1.01	0.84	4
OG--HG	1.01	0.84	15
OG--HG	1.02	0.84	9

Standard geometry: angle outliers

There are 122 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
CB-CG-CD2	131.20	121.18	1
CB-CG-CD2	131.20	121.21	1
CB-CG-CD2	131.20	121.24	1
CB-CG-CD2	131.20	121.25	1
CA-CB-CG	112.60	119.41	1
CA-CB-CG	112.60	119.40	1
CA-CB-CG	112.60	119.38	2
CD-NE-CZ	124.40	133.78	1
CD-NE-CZ	124.40	133.75	1
CD-NE-CZ	124.40	133.73	2
C-N-CA	121.70	133.66	1
C-N-CA	121.70	133.59	3
CD-NE-CZ	124.40	132.76	1
CD-NE-CZ	124.40	132.73	1
CD-NE-CZ	124.40	132.70	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-NE-CZ	124.40	132.67	1
CA-CB-CG	113.80	108.03	1
CA-CB-CG	113.80	108.04	1
CA-CB-CG	113.80	108.08	1
CA-CB-CG	113.80	108.11	1
C-CA-CB	110.10	120.50	1
C-CA-CB	110.10	120.49	1
C-CA-CB	110.10	120.48	1
C-N-CA	121.70	131.52	1
C-N-CA	121.70	131.51	1
C-CA-CB	110.10	120.45	1
C-N-CA	121.70	131.48	1
CB-CG-CD2	131.20	124.18	1
C-N-CA	121.70	131.40	1
CB-CG-CD2	131.20	124.20	1
CB-CG-CD2	131.20	124.22	1
CB-CG-CD2	131.20	124.23	1
C-CA-CB	111.60	122.07	1
C-CA-CB	111.60	122.05	2
C-CA-CB	111.60	122.01	1
CB-CG-CD2	131.20	124.44	1
CB-CG-CD2	131.20	124.47	1
CB-CG-CD2	131.20	124.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	124.50	1
CA-CB-CG	113.80	108.76	2
CA-CB-CG	113.80	108.78	1
C-N-CA	121.70	130.69	1
C-N-CA	121.70	130.68	1
C-N-CA	121.70	130.63	1
C-N-CA	121.70	130.60	1
CA-CB-CG	113.80	108.87	1
CB-CG-CD2	131.20	124.88	1
CB-CG-CD2	131.20	124.92	1
CB-CG-CD2	131.20	124.94	1
CB-CG-CD2	131.20	125.00	1
NE-CZ-NH1	121.50	126.13	1
NE-CZ-NH1	121.50	126.10	1
NE-CZ-NH1	121.50	126.08	1
NE-CZ-NH1	121.50	126.05	1
CA-CB-CG	112.60	117.13	1
OE1-CD-NE2	122.60	118.08	1
OE1-CD-NE2	122.60	118.10	3
CA-CB-CG	112.60	117.09	1
CA-CB-CG	112.60	117.06	1
CA-CB-CG	112.60	117.05	1
CA-CB-CG1	110.40	117.88	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.53	2
CA-CB-CG1	110.40	117.81	1
CB-CG-CD2	131.20	125.54	1
CA-CB-CG1	110.40	117.80	1
CA-CB-CG1	110.40	117.79	1
CA-CB-CG	113.80	118.11	1
N-CA-CB	103.00	107.73	1
CB-CG-CD2	131.20	125.62	1
N-CA-CB	103.00	107.72	1
CA-CB-CG	113.80	118.08	2
N-CA-CB	103.00	107.71	1
CA-CB-CG	113.80	118.06	1
N-CA-CB	103.00	107.68	1
OD1-CG-ND2	122.60	118.35	1
OD1-CG-ND2	122.60	118.37	2
OD1-CG-ND2	122.60	118.38	1
CA-CB-CG	113.80	118.01	1
OE1-CD-NE2	122.60	118.40	2
CA-CB-CG	113.80	117.98	2
C-N-CA	121.70	129.21	3
C-N-CA	121.70	129.20	1
CB-CG-CD2	131.20	125.79	2
OE1-CD-NE2	122.60	118.45	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.80	1
CA-CB-CG	113.80	117.94	1
CD1-CG-CD2	110.80	101.72	1
CD1-CG-CD2	110.80	101.73	1
CB-CG-CD2	131.20	125.85	1
CD1-CG-CD2	110.80	101.75	2
OE1-CD-NE2	122.60	118.49	1
OE1-CD-NE2	122.60	118.50	1
OE1-CD-NE2	122.60	118.51	1
CD-NE-CZ	124.40	130.11	1
OE1-CD-NE2	122.60	118.54	1
CB-CG-CD2	131.20	125.92	1
CB-CG-CD2	131.20	125.94	1
OE1-CD-NE2	122.60	118.56	1
CD-NE-CZ	124.40	130.05	1
CD-NE-CZ	124.40	130.04	1
CB-CG-CD2	131.20	125.97	1
CD1-CG-CD2	110.80	101.95	1
CB-CG-CD2	131.20	125.98	1
CA-CB-CG	112.60	116.61	1
CD1-CG-CD2	110.80	102.00	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	7.25	44
2	8.23	50
3	7.08	43
4	8.07	49

All 186 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:473:ALA:HB2	A:488:ILE:HB	1.031
1	A:431:PHE:HB3	A:462:VAL:HB	0.847
1	A:448:LEU:HD23	A:451:ALA:HB3	0.786
1	A:338:ILE:HD11	A:359:ILE:HD11	0.734
1	A:360:LEU:HB2	A:389:ILE:HG22	0.731
1	A:473:ALA:CB	A:488:ILE:HB	0.711
1	A:473:ALA:HB2	A:488:ILE:CB	0.684
1	A:452:LEU:HD11	A:475:ARG:HB2	0.672
1	A:337:PHE:CE2	A:358:GLN:HG2	0.663
1	A:525:THR:HG23	A:724:LEU:HD12	0.637
1	A:539:ILE:HG22	A:540:LEU:H	0.629
1	A:336:ILE:HG21	A:375:ALA:HB2	0.627
1	A:431:PHE:HD2	A:462:VAL:HG11	0.619
1	A:475:ARG:HE	A:482:THR:HG21	0.567
1	A:428:LYS:HB2	A:721:ARG:HH22	0.562
1	A:360:LEU:HB2	A:389:ILE:CG2	0.557
1	A:431:PHE:CD2	A:462:VAL:HG11	0.546

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:463:ILE:HB	A:472:GLN:HB3	0.542
1	A:525:THR:CG2	A:724:LEU:HD12	0.490
1	A:395:GLU:O	A:396:GLU:C	0.489
1	A:526:VAL:HB	A:717:TRP:CB	0.486
1	A:329:GLY:HA2	A:336:ILE:HG22	0.483
1	A:526:VAL:HB	A:717:TRP:HB3	0.482
1	A:336:ILE:HG13	A:359:ILE:HB	0.475
1	A:452:LEU:HB2	A:486:GLY:HA3	0.469
1	A:656:GLU:CD	A:656:GLU:H	0.469
1	A:436:LEU:HD12	A:686:GLU:HA	0.455
1	A:439:TYR:HE2	A:448:LEU:HD21	0.449
1	A:452:LEU:HD11	A:475:ARG:CB	0.449
1	A:433:ILE:HG22	A:460:LEU:HB2	0.448
1	A:502:LEU:HA	A:502:LEU:HD12	0.448
1	A:316:ILE:HD12	A:325:PHE:HE2	0.445
1	A:349:LEU:O	A:350:SER:C	0.438
1	A:459:VAL:HG11	A:717:TRP:CD1	0.438
1	A:435:ALA:HB2	A:454:PHE:HE2	0.434
1	A:431:PHE:HA	A:431:PHE:HD1	0.429
1	A:436:LEU:HA	A:456:PHE:CE1	0.420
1	A:475:ARG:NE	A:482:THR:HG21	0.416
1	A:455:ARG:H	A:455:ARG:HG2	0.409
1	A:464:ASP:HB3	A:465:ALA:H	0.407

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:719:PRO:HB3	A:720:ALA:H	0.405
1	A:431:PHE:HB3	A:462:VAL:CB	0.403
1	A:443:LYS:HD2	A:452:LEU:HA	0.402
1	A:325:PHE:HD2	A:347:ALA:HB2	0.402
2	A:473:ALA:HB2	A:488:ILE:HB	1.032
2	A:351:GLY:HA3	A:500:SER:OG	0.874
2	A:431:PHE:HB3	A:462:VAL:HB	0.849
2	A:448:LEU:HD23	A:451:ALA:HB3	0.786
2	A:338:ILE:HD11	A:359:ILE:HD11	0.750
2	A:360:LEU:HB2	A:389:ILE:HG22	0.736
2	A:473:ALA:CB	A:488:ILE:HB	0.712
2	A:473:ALA:HB2	A:488:ILE:CB	0.684
2	A:452:LEU:HD11	A:475:ARG:HB2	0.671
2	A:337:PHE:CE2	A:358:GLN:HG2	0.660
2	A:525:THR:HG23	A:724:LEU:HD12	0.637
2	A:539:ILE:HG22	A:540:LEU:H	0.631
2	A:431:PHE:HD2	A:462:VAL:HG11	0.619
2	A:336:ILE:HG21	A:375:ALA:HB2	0.618
2	A:475:ARG:HE	A:482:THR:HG21	0.568
2	A:354:ARG:HE	A:503:LYS:HG2	0.566
2	A:428:LYS:HB2	A:721:ARG:HH22	0.562
2	A:360:LEU:HB2	A:389:ILE:CG2	0.548
2	A:431:PHE:CD2	A:462:VAL:HG11	0.547

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:463:ILE:HB	A:472:GLN:HB3	0.542
2	A:395:GLU:O	A:396:GLU:C	0.530
2	A:525:THR:CG2	A:724:LEU:HD12	0.491
2	A:491:LYS:H	A:491:LYS:HG3	0.487
2	A:526:VAL:HB	A:717:TRP:CB	0.486
2	A:526:VAL:HB	A:717:TRP:HB3	0.482
2	A:329:GLY:HA2	A:336:ILE:HG22	0.478
2	A:354:ARG:NE	A:503:LYS:HG2	0.476
2	A:336:ILE:HG13	A:359:ILE:HB	0.473
2	A:452:LEU:HB2	A:486:GLY:HA3	0.471
2	A:656:GLU:CD	A:656:GLU:H	0.470
2	A:316:ILE:HD12	A:325:PHE:HE2	0.462
2	A:436:LEU:HD12	A:686:GLU:HA	0.454
2	A:343:ALA:HB2	A:505:LYS:HE2	0.450
2	A:439:TYR:HE2	A:448:LEU:HD21	0.448
2	A:452:LEU:HD11	A:475:ARG:CB	0.448
2	A:433:ILE:HG22	A:460:LEU:HB2	0.447
2	A:502:LEU:HA	A:502:LEU:HD12	0.447
2	A:349:LEU:O	A:350:SER:C	0.441
2	A:459:VAL:HG11	A:717:TRP:CD1	0.438
2	A:435:ALA:HB2	A:454:PHE:HE2	0.434
2	A:338:ILE:HD11	A:359:ILE:CD1	0.423
2	A:431:PHE:HA	A:431:PHE:HD1	0.423

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:436:LEU:HA	A:456:PHE:CE1	0.420
2	A:475:ARG:NE	A:482:THR:HG21	0.417
2	A:455:ARG:H	A:455:ARG:HG2	0.410
2	A:325:PHE:HD2	A:347:ALA:HB2	0.405
2	A:464:ASP:HB3	A:465:ALA:H	0.405
2	A:431:PHE:HB3	A:462:VAL:CB	0.404
2	A:443:LYS:HD2	A:452:LEU:HA	0.404
2	A:719:PRO:HB3	A:720:ALA:H	0.404
3	A:473:ALA:HB2	A:488:ILE:HB	1.030
3	A:431:PHE:HB3	A:462:VAL:HB	0.848
3	A:448:LEU:HD23	A:451:ALA:HB3	0.787
3	A:338:ILE:HD11	A:359:ILE:HD11	0.747
3	A:360:LEU:HB2	A:389:ILE:HG22	0.735
3	A:473:ALA:CB	A:488:ILE:HB	0.711
3	A:473:ALA:HB2	A:488:ILE:CB	0.683
3	A:452:LEU:HD11	A:475:ARG:HB2	0.673
3	A:337:PHE:CE2	A:358:GLN:HG2	0.663
3	A:525:THR:HG23	A:724:LEU:HD12	0.638
3	A:539:ILE:HG22	A:540:LEU:H	0.631
3	A:431:PHE:HD2	A:462:VAL:HG11	0.621
3	A:336:ILE:HG21	A:375:ALA:HB2	0.616
3	A:475:ARG:HE	A:482:THR:HG21	0.568
3	A:428:LYS:HB2	A:721:ARG:HH22	0.562

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:431:PHE:CD2	A:462:VAL:HG11	0.547
3	A:463:ILE:HB	A:472:GLN:HB3	0.542
3	A:360:LEU:HB2	A:389:ILE:CG2	0.538
3	A:395:GLU:O	A:396:GLU:C	0.521
3	A:525:THR:CG2	A:724:LEU:HD12	0.491
3	A:526:VAL:HB	A:717:TRP:CB	0.486
3	A:526:VAL:HB	A:717:TRP:HB3	0.482
3	A:336:ILE:HG13	A:359:ILE:HB	0.475
3	A:656:GLU:CD	A:656:GLU:H	0.471
3	A:329:GLY:HA2	A:336:ILE:HG22	0.468
3	A:452:LEU:HB2	A:486:GLY:HA3	0.467
3	A:316:ILE:HD12	A:325:PHE:HE2	0.456
3	A:436:LEU:HD12	A:686:GLU:HA	0.454
3	A:439:TYR:HE2	A:448:LEU:HD21	0.449
3	A:452:LEU:HD11	A:475:ARG:CB	0.449
3	A:502:LEU:HA	A:502:LEU:HD12	0.447
3	A:433:ILE:HG22	A:460:LEU:HB2	0.446
3	A:459:VAL:HG11	A:717:TRP:CD1	0.438
3	A:435:ALA:HB2	A:454:PHE:HE2	0.434
3	A:349:LEU:O	A:350:SER:C	0.433
3	A:431:PHE:HA	A:431:PHE:HD1	0.430
3	A:436:LEU:HA	A:456:PHE:CE1	0.421
3	A:475:ARG:NE	A:482:THR:HG21	0.417

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:455:ARG:H	A:455:ARG:HG2	0.412
3	A:464:ASP:HB3	A:465:ALA:H	0.406
3	A:719:PRO:HB3	A:720:ALA:H	0.405
3	A:431:PHE:HB3	A:462:VAL:CB	0.403
3	A:443:LYS:HD2	A:452:LEU:HA	0.403
4	A:349:LEU:HD21	A:633:ASN:OD1	1.036
4	A:473:ALA:HB2	A:488:ILE:HB	1.030
4	A:431:PHE:HB3	A:462:VAL:HB	0.849
4	A:448:LEU:HD23	A:451:ALA:HB3	0.787
4	A:338:ILE:HD11	A:359:ILE:HD11	0.741
4	A:360:LEU:HB2	A:389:ILE:HG22	0.720
4	A:473:ALA:CB	A:488:ILE:HB	0.711
4	A:473:ALA:HB2	A:488:ILE:CB	0.683
4	A:452:LEU:HD11	A:475:ARG:HB2	0.673
4	A:337:PHE:CE2	A:358:GLN:HG2	0.657
4	A:525:THR:HG23	A:724:LEU:HD12	0.638
4	A:539:ILE:HG22	A:540:LEU:H	0.632
4	A:336:ILE:HG21	A:375:ALA:HB2	0.623
4	A:431:PHE:HD2	A:462:VAL:HG11	0.621
4	A:349:LEU:HD21	A:633:ASN:CG	0.592
4	A:475:ARG:HE	A:482:THR:HG21	0.567
4	A:428:LYS:HB2	A:721:ARG:HH22	0.563
4	A:431:PHE:CD2	A:462:VAL:HG11	0.548

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:463:ILE:HB	A:472:GLN:HB3	0.544
4	A:360:LEU:HB2	A:389:ILE:CG2	0.543
4	A:525:THR:CG2	A:724:LEU:HD12	0.491
4	A:395:GLU:O	A:396:GLU:C	0.489
4	A:491:LYS:H	A:491:LYS:HG3	0.487
4	A:526:VAL:HB	A:717:TRP:CB	0.485
4	A:526:VAL:HB	A:717:TRP:HB3	0.481
4	A:329:GLY:HA2	A:336:ILE:HG22	0.473
4	A:336:ILE:HG13	A:359:ILE:HB	0.473
4	A:452:LEU:HB2	A:486:GLY:HA3	0.470
4	A:656:GLU:CD	A:656:GLU:H	0.469
4	A:436:LEU:HD12	A:686:GLU:HA	0.454
4	A:439:TYR:HE2	A:448:LEU:HD21	0.449
4	A:452:LEU:HD11	A:475:ARG:CB	0.449
4	A:433:ILE:HG22	A:460:LEU:HB2	0.447
4	A:502:LEU:HA	A:502:LEU:HD12	0.446
4	A:316:ILE:HD12	A:325:PHE:HE2	0.443
4	A:459:VAL:HG11	A:717:TRP:CD1	0.438
4	A:349:LEU:O	A:350:SER:C	0.434
4	A:435:ALA:HB2	A:454:PHE:HE2	0.433
4	A:338:ILE:HD11	A:359:ILE:CD1	0.432
4	A:431:PHE:HA	A:431:PHE:HD1	0.422
4	A:436:LEU:HA	A:456:PHE:CE1	0.420

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:349:LEU:CD2	A:633:ASN:OD1	0.417
4	A:475:ARG:NE	A:482:THR:HG21	0.416
4	A:455:ARG:H	A:455:ARG:HG2	0.409
4	A:464:ASP:HB3	A:465:ALA:H	0.405
4	A:719:PRO:HB3	A:720:ALA:H	0.405
4	A:431:PHE:HB3	A:462:VAL:CB	0.404
4	A:443:LYS:HD2	A:452:LEU:HA	0.404
4	A:393:LYS:HA	A:394:PRO:HD3	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	379	334	33	12
2	379	335	32	12
3	379	334	33	12
4	379	335	32	12

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	327	219	51	57
2	327	219	52	56
3	327	219	51	57
4	327	219	51	57

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	316	ILE
1	A	318	ARG
1	A	323	LEU
1	A	327	ILE
1	A	346	PRO
1	A	350	SER
1	A	369	ASN
1	A	371	SER
1	A	374	GLN
1	A	379	LEU
1	A	384	GLN
1	A	386	VAL
1	A	387	THR
1	A	389	ILE
1	A	431	PHE
1	A	437	PHE
1	A	438	ASP
1	A	445	CYS
1	A	449	SER
1	A	458	ASP
1	A	459	VAL
1	A	464	ASP
1	A	470	TRP

Model ID	Chain	Residue ID	Residue type
1	A	474	ARG
1	A	481	GLU
1	A	482	THR
1	A	483	ASP
1	A	491	LYS
1	A	494	VAL
1	A	497	ARG
1	A	502	LEU
1	A	514	GLN
1	A	520	VAL
1	A	521	LEU
1	A	525	THR
1	A	526	VAL
1	A	527	THR
1	A	544	LYS
1	A	545	ASP
1	A	567	THR
1	A	590	GLU
1	A	596	HIS
1	A	605	ASN
1	A	617	ARG
1	A	618	GLU
1	A	624	LYS

Model ID	Chain	Residue ID	Residue type
1	A	629	ASP
1	A	671	ARG
1	A	679	LYS
1	A	685	THR
1	A	686	GLU
1	A	687	CYS
1	A	716	ILE
1	A	718	VAL
1	A	721	ARG
1	A	723	ARG
1	A	724	LEU
2	A	316	ILE
2	A	318	ARG
2	A	323	LEU
2	A	327	ILE
2	A	346	PRO
2	A	350	SER
2	A	369	ASN
2	A	371	SER
2	A	374	GLN
2	A	379	LEU
2	A	384	GLN
2	A	386	VAL

Model ID	Chain	Residue ID	Residue type
2	A	387	THR
2	A	389	ILE
2	A	431	PHE
2	A	437	PHE
2	A	438	ASP
2	A	445	CYS
2	A	449	SER
2	A	458	ASP
2	A	459	VAL
2	A	464	ASP
2	A	470	TRP
2	A	474	ARG
2	A	481	GLU
2	A	482	THR
2	A	491	LYS
2	A	494	VAL
2	A	497	ARG
2	A	502	LEU
2	A	514	GLN
2	A	520	VAL
2	A	521	LEU
2	A	525	THR
2	A	526	VAL

Model ID	Chain	Residue ID	Residue type
2	A	527	THR
2	A	544	LYS
2	A	545	ASP
2	A	567	THR
2	A	590	GLU
2	A	596	HIS
2	A	605	ASN
2	A	617	ARG
2	A	618	GLU
2	A	624	LYS
2	A	629	ASP
2	A	671	ARG
2	A	679	LYS
2	A	685	THR
2	A	686	GLU
2	A	687	CYS
2	A	716	ILE
2	A	718	VAL
2	A	721	ARG
2	A	723	ARG
2	A	724	LEU
3	A	316	ILE
3	A	318	ARG

Model ID	Chain	Residue ID	Residue type
3	A	323	LEU
3	A	327	ILE
3	A	346	PRO
3	A	350	SER
3	A	369	ASN
3	A	371	SER
3	A	374	GLN
3	A	379	LEU
3	A	384	GLN
3	A	386	VAL
3	A	387	THR
3	A	389	ILE
3	A	431	PHE
3	A	437	PHE
3	A	438	ASP
3	A	445	CYS
3	A	449	SER
3	A	458	ASP
3	A	459	VAL
3	A	464	ASP
3	A	470	TRP
3	A	474	ARG
3	A	481	GLU

Model ID	Chain	Residue ID	Residue type
3	A	482	THR
3	A	483	ASP
3	A	491	LYS
3	A	494	VAL
3	A	497	ARG
3	A	502	LEU
3	A	514	GLN
3	A	520	VAL
3	A	521	LEU
3	A	525	THR
3	A	526	VAL
3	A	527	THR
3	A	544	LYS
3	A	545	ASP
3	A	567	THR
3	A	590	GLU
3	A	596	HIS
3	A	605	ASN
3	A	617	ARG
3	A	618	GLU
3	A	624	LYS
3	A	629	ASP
3	A	671	ARG

Model ID	Chain	Residue ID	Residue type
3	A	679	LYS
3	A	685	THR
3	A	686	GLU
3	A	687	CYS
3	A	716	ILE
3	A	718	VAL
3	A	721	ARG
3	A	723	ARG
3	A	724	LEU
4	A	316	ILE
4	A	318	ARG
4	A	323	LEU
4	A	327	ILE
4	A	346	PRO
4	A	350	SER
4	A	369	ASN
4	A	371	SER
4	A	374	GLN
4	A	379	LEU
4	A	384	GLN
4	A	386	VAL
4	A	387	THR
4	A	389	ILE

Model ID	Chain	Residue ID	Residue type
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	483	ASP
4	A	491	LYS
4	A	494	VAL
4	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

Model ID	Chain	Residue ID	Residue type
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	724	LEU

Fit of model to data used for modeling

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.

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