Integrative Structure Validation Report

July 22, 2024 - 04:42 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	9A1Q
PDB-Dev ID	PDBDEV_00000098
Structure Title	The structural models of alpha-synuclein dimer
Structure Authors	Zamel J; Chen J; Zaer S; Harris PD; Drori P; Lebendiker M; Kalisman N; Dokholyan NV; Lerner 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

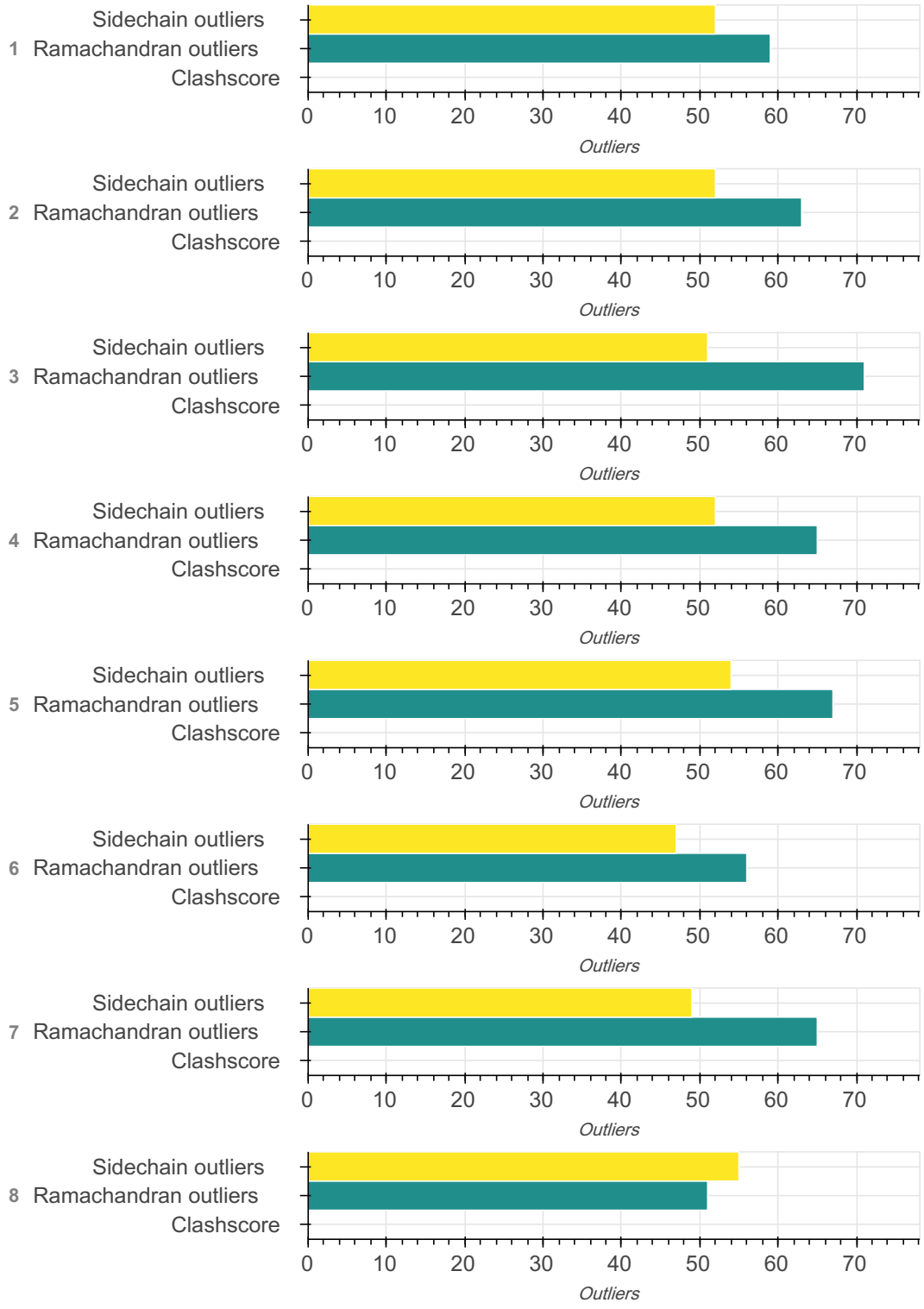
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 8 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 8 unique types of models in this entry.These models are titled None, None, None, None, None, None, None, None respectively.

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

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

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	PXD030299
2	De Novo model	Not available	Not available

Representation

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

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-140
B	-	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	Design square-well functions based on cross-linking constraints	At this step, cross-linking constraints are collected from experiments and used to design square-well functions for DMD simulations.	None	False	False
2	1	None	Perform DMD simulations	At this step, the designed square-well functions are incorporated into the force field. Start DMD simulations.	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	DMD software	Not available	model building	http://www.moleculesinaction.com/pdmd.html

Data quality

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 2896 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--HZ1	0.98	0.89	50
NZ--HZ2	0.98	0.89	49
NZ--HZ3	0.98	0.89	43
NZ--HZ1	0.99	0.89	84
NZ--HZ2	0.99	0.89	73
NZ--HZ3	0.99	0.89	83
NZ--HZ3	1.00	0.89	64
NZ--HZ1	1.00	0.89	68
NZ--HZ2	1.00	0.89	62
NZ--HZ3	1.01	0.89	41
NZ--HZ2	1.01	0.89	41
N--H	0.98	0.86	152
NZ--HZ1	1.01	0.89	27
N--H	0.99	0.86	372
NZ--HZ1	1.02	0.89	7
NZ--HZ3	1.02	0.89	7
NZ--HZ2	1.02	0.89	12
ND1--HD1	0.99	0.86	3
N--H	1.00	0.86	573
ND1--HD1	1.00	0.86	6
N--H	1.01	0.86	705
ND1--HD1	1.01	0.86	5
N--H	1.02	0.86	358

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND1--HD1	1.02	0.86	2
NZ--HZ2	1.72	0.89	1
NZ--HZ1	1.73	0.89	1
NZ--HZ2	1.73	0.89	1
NZ--HZ1	1.74	0.89	1
NZ--HZ1	1.75	0.89	1
NZ--HZ3	1.75	0.89	1
NZ--HZ3	1.76	0.89	1
NZ--HZ1	1.77	0.89	1
NZ--HZ2	1.77	0.89	1

Standard geometry: angle outliers

There are 50 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
CA-CB-CG	112.60	117.54	1
CA-CB-CG	112.60	116.99	1
CD1-CG-CD2	110.80	101.18	1
CD1-CG-CD2	110.80	101.31	1
CA-C-O	120.80	113.62	1
OD1-CG-ND2	122.60	118.39	1
CA-CB-CG2	110.40	117.56	2
CD1-CG-CD2	110.80	101.54	1
CD1-CG-CD2	110.80	101.65	1
CA-C-O	120.80	113.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD1-CG-CD2	110.80	101.70	1
CA-CB-CG2	110.40	117.41	1
CD1-CG-CD2	110.80	101.74	1
CA-CB-CG	112.60	116.72	1
CD1-CG-CD2	110.80	101.76	1
CD1-CG-CD2	110.80	101.78	1
CA-CB-CG	112.60	116.69	1
CA-CB-CG1	110.40	117.35	1
CD1-CG-CD2	110.80	101.82	1
CA-CB-CG2	110.40	117.26	1
CD1-CG-CD2	110.80	101.93	1
CA-N-H	126.74	114.00	1
CE-NZ-HZ2	77.99	110.00	1
CE-NZ-HZ3	77.92	110.00	1
CE-NZ-HZ1	77.29	110.00	1
CE-NZ-HZ3	76.78	110.00	1
CE-NZ-HZ1	76.69	110.00	1
CE-NZ-HZ2	76.36	110.00	1
CE-NZ-HZ1	75.87	110.00	1
CE-NZ-HZ1	75.83	110.00	1
CE-NZ-HZ2	75.78	110.00	1
HZ1-NZ-HZ2	69.54	109.00	1
HZ1-NZ-HZ2	68.41	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HZ2-NZ-HZ3	67.63	109.00	1
HZ1-NZ-HZ3	67.21	109.00	1
HZ1-NZ-HZ3	67.19	109.00	1
HZ2-NZ-HZ3	67.05	109.00	1
HZ1-NZ-HZ3	67.05	109.00	1
HZ1-NZ-HZ3	67.03	109.00	1
HZ2-NZ-HZ3	66.75	109.00	1
HZ1-NZ-HZ2	66.73	109.00	1
HZ2-NZ-HZ3	66.31	109.00	1
HZ1-NZ-HZ3	65.88	109.00	1
HZ1-NZ-HZ2	65.77	109.00	1
HZ1-NZ-HZ2	65.75	109.00	1
HZ1-NZ-HZ3	65.69	109.00	1
HZ1-NZ-HZ2	65.65	109.00	1
HZ1-NZ-HZ2	65.50	109.00	1
HZ2-NZ-HZ3	64.88	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	0.00	0
2	0.00	0
3	0.00	0

Model ID	Clash score	Number of clashes
4	0.00	0
5	0.00	0
6	0.00	0
7	0.00	0
8	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	276	162	55	59
2	276	159	54	63
3	276	157	48	71
4	276	167	44	65
5	276	160	49	67
6	276	161	59	56
7	276	152	59	65
8	276	168	57	51

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	206	120	34	52
2	206	113	41	52
3	206	125	30	51

Model ID	Analyzed	Favored	Allowed	Outliers
4	206	110	44	52
5	206	120	32	54
6	206	126	33	47
7	206	112	45	49
8	206	118	33	55

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	9	0SER
1	A	12	0LYS
1	A	32	0LYS
1	A	34	0LYS
1	A	38	0LEU
1	A	40	0VAL
1	A	42	0SER
1	A	46	0GLU
1	A	52	0VAL
1	A	59	0THR
1	A	63	0VAL
1	A	66	0VAL
1	A	71	0VAL
1	A	81	0THR
1	A	82	0VAL
1	A	94	0PHE

Model ID	Chain	Residue ID	Residue type
1	A	98	0ASP
1	A	100	0LEU
1	A	103	0ASN
1	A	112	0ILE
1	A	115	0ASP
1	A	121	0ASP
1	A	122	0ASN
1	A	126	0GLU
1	A	130	0GLU
1	B	2	0ASP
1	B	3	0VAL
1	B	4	0PHE
1	B	5	0MET
1	B	8	0LEU
1	B	16	0VAL
1	B	26	0VAL
1	B	33	0THR
1	B	38	0LEU
1	B	40	0VAL
1	B	49	0VAL
1	B	60	0LYS
1	B	62	0GLN
1	B	63	0VAL

Model ID	Chain	Residue ID	Residue type
1	B	64	0THR
1	B	66	0VAL
1	B	71	0VAL
1	B	72	0THR
1	B	79	0GLN
1	B	88	0ILE
1	B	92	0THR
1	B	97	0LYS
1	B	102	0LYS
1	B	109	0GLN
1	B	128	0PRO
1	B	134	0GLN
1	B	135	0ASP
2	A	2	0ASP
2	A	3	0VAL
2	A	16	0VAL
2	A	21	0LYS
2	A	33	0THR
2	A	34	0LYS
2	A	40	0VAL
2	A	42	0SER
2	A	43	0LYS
2	A	49	0VAL

Model ID	Chain	Residue ID	Residue type
2	A	59	0THR
2	A	64	0THR
2	A	65	0ASN
2	A	71	0VAL
2	A	72	0THR
2	A	75	0THR
2	A	77	0VAL
2	A	81	0THR
2	A	99	0GLN
2	A	109	0GLN
2	A	115	0ASP
2	A	118	0VAL
2	A	121	0ASP
2	A	123	0GLU
2	A	127	0MET
2	A	129	0SER
2	B	8	0LEU
2	B	9	0SER
2	B	10	0LYS
2	B	16	0VAL
2	B	21	0LYS
2	B	22	0THR
2	B	24	0GLN

Model ID	Chain	Residue ID	Residue type
2	B	37	0VAL
2	B	40	0VAL
2	B	43	0LYS
2	B	44	0THR
2	B	49	0VAL
2	B	59	0THR
2	B	63	0VAL
2	B	71	0VAL
2	B	74	0VAL
2	B	75	0THR
2	B	82	0VAL
2	B	83	0GLU
2	B	88	0ILE
2	B	98	0ASP
2	B	104	0GLU
2	B	112	0ILE
2	B	113	0LEU
2	B	115	0ASP
2	B	129	0SER
3	A	4	0PHE
3	A	8	0LEU
3	A	15	0VAL
3	A	33	0THR

Model ID	Chain	Residue ID	Residue type
3	A	34	0LYS
3	A	38	0LEU
3	A	39	0TYR
3	A	45	0LYS
3	A	46	0GLU
3	A	48	0VAL
3	A	54	0THR
3	A	55	0VAL
3	A	58	0LYS
3	A	63	0VAL
3	A	70	0VAL
3	A	75	0THR
3	A	88	0ILE
3	A	92	0THR
3	A	97	0LYS
3	A	102	0LYS
3	A	112	0ILE
3	A	118	0VAL
3	A	119	0ASP
3	A	121	0ASP
3	A	122	0ASN
3	A	137	0GLU
3	B	3	0VAL

Model ID	Chain	Residue ID	Residue type
3	B	16	0VAL
3	B	21	0LYS
3	B	22	0THR
3	B	26	0VAL
3	B	34	0LYS
3	B	38	0LEU
3	B	40	0VAL
3	B	48	0VAL
3	B	55	0VAL
3	B	59	0THR
3	B	60	0LYS
3	B	62	0GLN
3	B	71	0VAL
3	B	79	0GLN
3	B	81	0THR
3	B	82	0VAL
3	B	92	0THR
3	B	95	0VAL
3	B	109	0GLN
3	B	118	0VAL
3	B	120	0PRO
3	B	122	0ASN
3	B	129	0SER

Model ID	Chain	Residue ID	Residue type
3	B	137	0GLU
4	A	2	0ASP
4	A	3	0VAL
4	A	8	0LEU
4	A	24	0GLN
4	A	34	0LYS
4	A	37	0VAL
4	A	38	0LEU
4	A	39	0TYR
4	A	40	0VAL
4	A	49	0VAL
4	A	59	0THR
4	A	60	0LYS
4	A	64	0THR
4	A	65	0ASN
4	A	71	0VAL
4	A	75	0THR
4	A	81	0THR
4	A	94	0PHE
4	A	95	0VAL
4	A	100	0LEU
4	A	104	0GLU
4	A	112	0ILE

Model ID	Chain	Residue ID	Residue type
4	A	115	0ASP
4	A	116	0MET
4	A	118	0VAL
4	A	121	0ASP
4	A	127	0MET
4	A	135	0ASP
4	B	1	0MET
4	B	2	0ASP
4	B	3	0VAL
4	B	15	0VAL
4	B	24	0GLN
4	B	26	0VAL
4	B	38	0LEU
4	B	44	0THR
4	B	49	0VAL
4	B	63	0VAL
4	B	64	0THR
4	B	71	0VAL
4	B	72	0THR
4	B	74	0VAL
4	B	77	0VAL
4	B	79	0GLN
4	B	95	0VAL

Model ID	Chain	Residue ID	Residue type
4	B	98	0ASP
4	B	102	0LYS
4	B	115	0ASP
4	B	133	0TYR
4	B	134	0GLN
4	B	135	0ASP
4	B	139	0GLU
5	A	2	0ASP
5	A	3	0VAL
5	A	8	0LEU
5	A	13	0GLU
5	A	24	0GLN
5	A	26	0VAL
5	A	33	0THR
5	A	34	0LYS
5	A	35	0GLU
5	A	38	0LEU
5	A	43	0LYS
5	A	46	0GLU
5	A	52	0VAL
5	A	57	0GLU
5	A	59	0THR
5	A	64	0THR

Model ID	Chain	Residue ID	Residue type
5	A	66	0VAL
5	A	71	0VAL
5	A	72	0THR
5	A	75	0THR
5	A	83	0GLU
5	A	87	0SER
5	A	88	0ILE
5	A	92	0THR
5	A	100	0LEU
5	A	105	0GLU
5	A	113	0LEU
5	A	116	0MET
5	A	118	0VAL
5	A	121	0ASP
5	A	133	0TYR
5	A	134	0GLN
5	B	8	0LEU
5	B	16	0VAL
5	B	21	0LYS
5	B	22	0THR
5	B	24	0GLN
5	B	26	0VAL
5	B	35	0GLU

Model ID	Chain	Residue ID	Residue type
5	B	37	0VAL
5	B	39	0TYR
5	B	46	0GLU
5	B	48	0VAL
5	B	63	0VAL
5	B	70	0VAL
5	B	71	0VAL
5	B	72	0THR
5	B	79	0GLN
5	B	94	0PHE
5	B	115	0ASP
5	B	120	0PRO
5	B	131	0GLU
5	B	133	0TYR
5	B	139	0GLU
6	A	13	0GLU
6	A	16	0VAL
6	A	26	0VAL
6	A	33	0THR
6	A	34	0LYS
6	A	38	0LEU
6	A	40	0VAL
6	A	43	0LYS

Model ID	Chain	Residue ID	Residue type
6	A	44	0THR
6	A	48	0VAL
6	A	49	0VAL
6	A	58	0LYS
6	A	59	0THR
6	A	72	0THR
6	A	75	0THR
6	A	77	0VAL
6	A	81	0THR
6	A	87	0SER
6	A	88	0ILE
6	A	112	0ILE
6	A	123	0GLU
6	A	127	0MET
6	A	133	0TYR
6	A	139	0GLU
6	B	1	0MET
6	B	15	0VAL
6	B	16	0VAL
6	B	21	0LYS
6	B	23	0LYS
6	B	26	0VAL
6	B	32	0LYS

Model ID	Chain	Residue ID	Residue type
6	B	37	0VAL
6	B	40	0VAL
6	B	42	0SER
6	B	54	0THR
6	B	55	0VAL
6	B	59	0THR
6	B	63	0VAL
6	B	79	0GLN
6	B	82	0VAL
6	B	88	0ILE
6	B	92	0THR
6	B	98	0ASP
6	B	100	0LEU
6	B	112	0ILE
6	B	116	0MET
6	B	133	0TYR
7	A	3	0VAL
7	A	4	0PHE
7	A	8	0LEU
7	A	9	0SER
7	A	12	0LYS
7	A	13	0GLU
7	A	26	0VAL

Model ID	Chain	Residue ID	Residue type
7	A	33	0THR
7	A	35	0GLU
7	A	43	0LYS
7	A	45	0LYS
7	A	46	0GLU
7	A	49	0VAL
7	A	50	0HIS
7	A	52	0VAL
7	A	55	0VAL
7	A	59	0THR
7	A	64	0THR
7	A	66	0VAL
7	A	70	0VAL
7	A	72	0THR
7	A	77	0VAL
7	A	88	0ILE
7	A	99	0GLN
7	A	113	0LEU
7	A	115	0ASP
7	A	130	0GLU
7	A	133	0TYR
7	A	135	0ASP
7	B	2	0ASP

Model ID	Chain	Residue ID	Residue type
7	B	10	0LYS
7	B	16	0VAL
7	B	28	0GLU
7	B	35	0GLU
7	B	38	0LEU
7	B	40	0VAL
7	B	48	0VAL
7	B	62	0GLN
7	B	71	0VAL
7	B	77	0VAL
7	B	81	0THR
7	B	88	0ILE
7	B	92	0THR
7	B	95	0VAL
7	B	100	0LEU
7	B	105	0GLU
7	B	121	0ASP
7	B	127	0MET
7	B	133	0TYR
8	A	12	0LYS
8	A	16	0VAL
8	A	20	0GLU
8	A	24	0GLN

Model ID	Chain	Residue ID	Residue type
8	A	26	0VAL
8	A	32	0LYS
8	A	37	0VAL
8	A	38	0LEU
8	A	39	0TYR
8	A	40	0VAL
8	A	43	0LYS
8	A	44	0THR
8	A	49	0VAL
8	A	50	0HIS
8	A	58	0LYS
8	A	63	0VAL
8	A	66	0VAL
8	A	70	0VAL
8	A	71	0VAL
8	A	72	0THR
8	A	83	0GLU
8	A	88	0ILE
8	A	94	0PHE
8	A	99	0GLN
8	A	103	0ASN
8	A	105	0GLU
8	A	112	0ILE

Model ID	Chain	Residue ID	Residue type
8	A	119	0ASP
8	A	128	0PRO
8	B	8	0LEU
8	B	9	0SER
8	B	15	0VAL
8	B	16	0VAL
8	B	26	0VAL
8	B	35	0GLU
8	B	39	0TYR
8	B	40	0VAL
8	B	44	0THR
8	B	48	0VAL
8	B	49	0VAL
8	B	54	0THR
8	B	64	0THR
8	B	79	0GLN
8	B	88	0ILE
8	B	92	0THR
8	B	94	0PHE
8	B	104	0GLU
8	B	112	0ILE
8	B	113	0LEU
8	B	114	0GLU

Model ID	Chain	Residue ID	Residue type
8	B	116	0MET
8	B	121	0ASP
8	B	127	0MET
8	B	135	0ASP
8	B	137	0GLU

Fit of model to data used for modeling

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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