

# Integrative Structure Validation Report ?

February 27, 2025 - 12:21 PM PST

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	9A8F
PDB-Dev ID	PDBDEV_00000379
Structure Title	Type II Amyloid beta Fibril MEMMI ensemble
Structure Authors	Milanesi, M.; Brotzakis, Z.F.; Vendruscolo, M.
Deposited on	2024-02-02

*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](mailto:helpdesk@pdb-ihm.org)

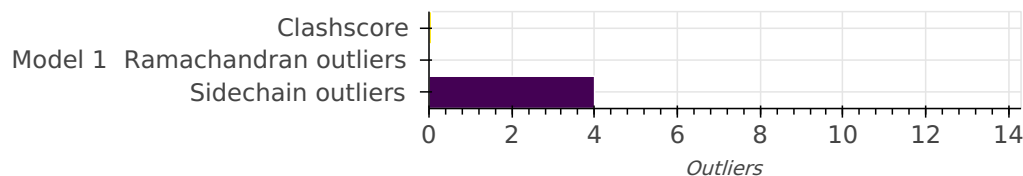
A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.

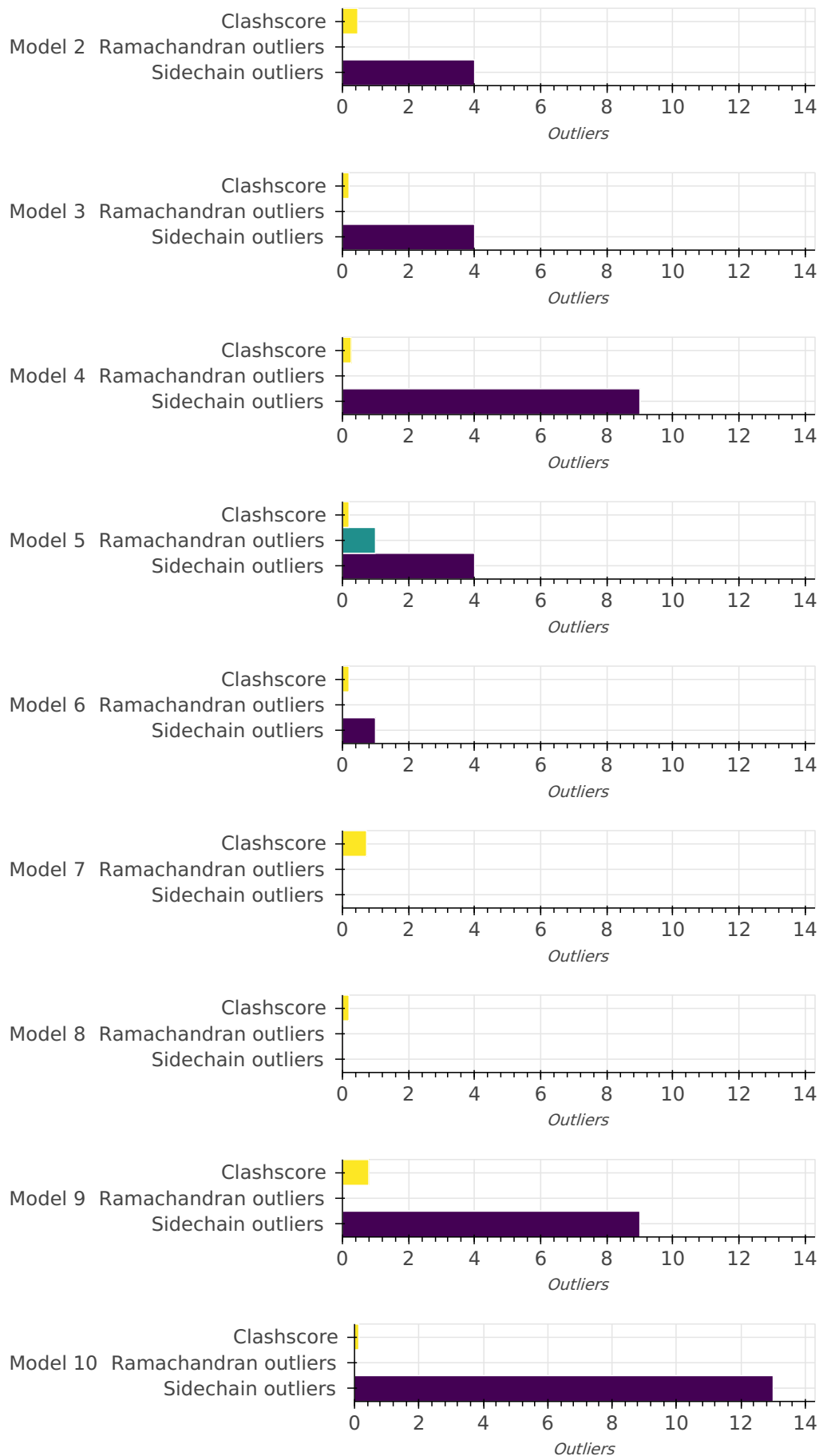
List of references used to build this report is available [here](#).

## 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 10 model(s). A total of 3 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
1	1-10	1	Amyloid-beta protein 42	A	42	-	1-42	100.00 / 100.00	Atomic
				B					
				C					
				D					
				E					
				F					
				G					
				H					
				I					
				J					
				K					
				L					
				M					
				N					
				O					
				P					
				Q					
				R					
				S					
				T					
				U					
				V					

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

### Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	Experimental model	PDB	7q4m
5	3DEM volume	Zenodo	<a href="https://zenodo.org/record/14766466">10.5281/zenodo.14766466</a>
1	3DEM volume	EMDB	EMD-13809

### 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	None	All the necessary input files for the ensemble generation are available at <a href="https://zenodo.org/records/14766466">https://zenodo.org/records/14766466</a> in the SIMULATION zip file.	None	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	<a href="#">gmmconvert</a>	Not available	express the experimental voxel map data as GMM data	<a href="https://gitlab.pasteur.fr/rpellari/recursive-gmconvert">https://gitlab.pasteur.fr/rpellari/recursive-gmconvert</a>
2	<a href="#">Gromacs</a>	GROMACS-2020.5	free and open-source software suite for high-performance molecular dynamics and output analysis	<a href="https://www.gromacs.org">https://www.gromacs.org</a>
3	<a href="#">Plumed</a>	PLUMED.2.6.0-dev	enhanced-sampling algorithms	<a href="https://github.com/tlhr/plumed2.git">https://github.com/tlhr/plumed2.git</a>

Data quality ?  
3DEM volume

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 89 bond length outliers in this entry (0.11% of 78000 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	24	VAL	C-O	26.41	0.70	1.23	5	2
B	24	VAL	C-N	24.85	0.98	1.33	5	2
W	15	GLN	C-O	22.31	0.78	1.23	6	1
B	11	GLU	C-O	16.05	0.91	1.23	5	1
V	12	VAL	C-O	15.96	0.91	1.23	6	1
W	15	GLN	C-N	15.46	1.11	1.33	6	1
B	11	GLU	C-N	13.53	1.14	1.33	5	1
L	24	VAL	C-O	11.96	0.99	1.23	5	1
P	24	VAL	C-O	11.93	0.99	1.23	5	2
P	24	VAL	C-N	11.16	1.17	1.33	5	2
V	40	VAL	C-O	11.01	1.01	1.23	5	1
T	20	PHE	C-O	10.83	1.01	1.23	6	1
L	24	VAL	C-N	10.61	1.18	1.33	5	1
W	16	LYS	CE-NZ	10.22	1.18	1.49	6	1
V	12	VAL	C-N	10.12	1.19	1.33	6	1
N	16	LYS	CE-NZ	9.90	1.19	1.49	6	1
D	24	VAL	C-N	8.83	1.21	1.33	9	1
V	40	VAL	C-N	8.78	1.21	1.33	5	1
D	24	VAL	C-O	8.66	1.06	1.23	9	2
D	26	SER	CB-OG	8.41	1.25	1.42	3	1
R	2	ALA	C-O	7.84	1.07	1.23	6	1
T	20	PHE	C-N	7.17	1.23	1.33	6	1
V	41	ILE	CG1-CD1	6.52	1.26	1.51	5	1
R	13	HIS	CG-CD2	6.32	1.42	1.35	10	1
P	9	GLY	C-O	6.19	1.11	1.23	6	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	24	VAL	CB-CG1	6.05	1.32	1.52	5	2
N	16	LYS	CG-CD	5.97	1.34	1.52	6	1
I	5	ARG	CZ-NH2	5.95	1.25	1.33	10	1
W	5	ARG	CD-NE	5.95	1.54	1.46	10	1
N	16	LYS	CD-CE	5.84	1.34	1.52	6	1
P	25	GLY	N-CA	5.80	1.36	1.45	5	1
D	24	VAL	CB-CG1	5.71	1.33	1.52	9	1
H	26	SER	C-N	5.71	1.41	1.33	9	1
W	29	GLY	C-N	5.70	1.41	1.33	9	1
D	10	TYR	CZ-OH	5.67	1.26	1.38	5	1
L	22	GLU	CD-OE1	5.66	1.14	1.25	1	1
C	37	GLY	CA-C	5.60	1.62	1.52	9	1
W	16	LYS	N-CA	5.45	1.35	1.46	6	1
S	41	ILE	CB-CG1	5.34	1.64	1.53	9	1
J	38	GLY	C-N	5.28	1.40	1.33	9	1
J	15	GLN	CD-OE1	5.22	1.13	1.23	4	1
W	6	HIS	CG-ND1	5.07	1.43	1.38	10	1
B	38	GLY	C-N	5.04	1.40	1.33	9	1
D	25	GLY	N-CA	5.02	1.53	1.45	10	1
I	38	GLY	N-CA	4.92	1.53	1.45	10	1
L	25	GLY	N-CA	4.91	1.37	1.45	5	1
P	4	PHE	CG-CD1	4.90	1.49	1.38	9	1
N	3	GLU	CD-OE2	4.88	1.34	1.25	9	1
H	32	ILE	CB-CG1	4.88	1.63	1.53	10	1
H	18	VAL	N-CA	4.72	1.55	1.46	9	1
P	9	GLY	C-N	4.68	1.26	1.33	6	1
G	15	GLN	CD-NE2	4.67	1.23	1.33	8	1
E	37	GLY	N-CA	4.65	1.53	1.45	9	1
B	27	ASN	CG-ND2	4.63	1.23	1.33	9	1
P	38	GLY	CA-C	4.61	1.60	1.52	9	1
B	1	ASP	CA-C	4.60	1.62	1.52	10	1
H	6	HIS	CE1-NE2	4.60	1.37	1.32	10	1
D	24	VAL	CB-CG2	4.58	1.37	1.52	9	1
I	24	VAL	CB-CG1	4.56	1.37	1.52	2	1
H	37	GLY	N-CA	4.51	1.52	1.45	9	2
W	5	ARG	CZ-NH2	4.42	1.27	1.33	10	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D	6	HIS	CG-ND1	4.41	1.43	1.38	10	1
P	41	ILE	CB-CG1	4.38	1.62	1.53	10	1
B	37	GLY	C-N	4.37	1.27	1.33	9	1
K	12	VAL	CB-CG1	4.35	1.38	1.52	5	1
J	38	GLY	CA-C	4.34	1.59	1.52	9	1
N	26	SER	CB-OG	4.34	1.33	1.42	2	1
E	25	GLY	N-CA	4.33	1.52	1.45	9	1
H	40	VAL	C-N	4.33	1.39	1.33	10	1
R	13	HIS	CE1-NE2	4.31	1.36	1.32	10	1
P	36	VAL	N-CA	4.29	1.54	1.46	9	1
R	13	HIS	ND1-CE1	4.24	1.36	1.32	10	1
K	12	VAL	C-O	4.24	1.15	1.23	5	1
N	7	ASP	N-CA	4.23	1.54	1.46	9	1
H	40	VAL	N-CA	4.19	1.54	1.46	9	1
V	41	ILE	CB-CG1	4.18	1.45	1.53	5	1
U	15	GLN	C-N	4.14	1.27	1.33	1	1
E	32	ILE	CA-C	4.13	1.61	1.52	10	1
R	41	ILE	N-CA	4.13	1.54	1.46	9	1
H	6	HIS	CD2-NE2	4.07	1.33	1.37	9	1
W	6	HIS	CD2-NE2	4.05	1.33	1.37	10	1
D	6	HIS	ND1-CE1	4.04	1.36	1.32	10	1

### Standard geometry: angle outliers ?

There are 805 bond angle outliers in this entry (0.77% of 104880 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	24	VAL	O-C-N	22.30	87.33	123.00	5	2
W	15	GLN	O-C-N	18.77	92.98	123.00	6	1
W	15	GLN	C-N-CA	16.81	151.95	121.70	6	1
B	11	GLU	O-C-N	13.30	101.72	123.00	5	1
W	15	GLN	CA-C-N	12.98	142.16	116.20	6	1
N	16	LYS	CG-CD-CE	11.91	138.69	111.30	6	1
B	11	GLU	C-N-CA	11.86	143.05	121.70	5	1
B	24	VAL	CA-C-N	11.78	139.76	116.20	5	2
P	24	VAL	O-C-N	11.58	104.47	123.00	5	2
B	24	VAL	C-N-CA	10.90	141.32	121.70	5	3
L	24	VAL	O-C-N	10.88	105.59	123.00	5	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	19	PHE	CA-CB-CG	10.85	102.95	113.80	9	2
B	11	GLU	CA-C-N	10.04	136.27	116.20	5	1
L	24	VAL	C-N-CA	9.33	138.49	121.70	5	1
N	16	LYS	CD-CE-NZ	9.11	141.04	111.90	6	1
X	14	HIS	CA-CB-CG	9.10	122.90	113.80	9	1
P	24	VAL	C-N-CA	9.05	137.99	121.70	5	2
V	12	VAL	O-C-N	8.85	108.84	123.00	6	1
J	27	ASN	OD1-CG-ND2	8.47	114.13	122.60	10	1
V	40	VAL	O-C-N	8.47	109.46	123.00	5	1
B	23	ASP	CA-CB-CG	8.30	120.90	112.60	10	4
V	41	ILE	CB-CG1-CD1	8.29	131.21	113.80	5	1
P	24	VAL	CA-C-N	8.21	132.63	116.20	5	1
V	40	VAL	C-N-CA	8.19	136.44	121.70	5	1
D	24	VAL	O-C-N	8.06	110.10	123.00	9	1
L	24	VAL	CA-C-N	7.99	132.18	116.20	5	1
J	27	ASN	CA-CB-CG	7.74	104.86	112.60	10	1
J	15	GLN	OE1-CD-NE2	7.63	114.97	122.60	4	2
D	6	HIS	CB-CG-CD2	7.48	121.47	131.20	10	5
V	12	VAL	CA-C-N	7.30	130.80	116.20	6	1
P	5	ARG	NE-CZ-NH1	7.26	128.76	121.50	9	1
W	2	ALA	C-CA-CB	7.16	121.23	110.50	10	1
R	15	GLN	OE1-CD-NE2	7.14	115.46	122.60	10	4
B	24	VAL	CA-C-O	7.12	132.91	120.80	5	1
V	40	VAL	CA-C-N	7.06	130.33	116.20	5	1
W	4	PHE	C-N-CA	6.98	134.27	121.70	6	1
S	39	VAL	CA-CB-CG1	6.94	122.19	110.40	10	1
L	5	ARG	CD-NE-CZ	6.84	133.98	124.40	9	1
N	16	LYS	CB-CG-CD	6.81	126.97	111.30	6	1
A	4	PHE	CA-CB-CG	6.75	120.55	113.80	10	1
P	11	GLU	CB-CG-CD	6.72	124.03	112.60	6	1
C	2	ALA	N-CA-CB	6.65	100.42	110.40	10	1
H	5	ARG	C-N-CA	6.61	133.59	121.70	9	1
A	23	ASP	CA-CB-CG	6.54	119.14	112.60	1	6
E	32	ILE	CA-CB-CG2	6.50	99.44	110.50	10	1
H	32	ILE	CA-CB-CG1	6.45	121.36	110.40	10	1
W	15	GLN	CA-CB-CG	6.44	126.97	114.10	6	1
W	27	ASN	CA-CB-CG	6.39	106.21	112.60	9	1



Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	4	PHE	C-N-CA	6.37	133.17	121.70	9	1
D	24	VAL	C-N-CA	6.35	133.14	121.70	9	1
I	6	HIS	CA-CB-CG	6.34	120.14	113.80	10	1
M	15	GLN	OE1-CD-NE2	6.30	116.30	122.60	10	3
R	23	ASP	CA-CB-CG	6.29	118.89	112.60	10	1
X	14	HIS	CB-CG-CD2	6.20	123.14	131.20	9	7
I	22	GLU	N-CA-CB	6.15	100.05	110.50	1	1
G	22	GLU	C-N-CA	6.08	132.65	121.70	10	1
T	41	ILE	CA-CB-CG2	6.06	100.20	110.50	9	1
W	16	LYS	CD-CE-NZ	6.04	131.24	111.90	6	1
H	22	GLU	C-N-CA	6.03	132.55	121.70	9	2
I	6	HIS	ND1-CG-CD2	6.03	112.13	106.10	10	1
W	16	LYS	CA-CB-CG	6.02	126.14	114.10	6	1
D	1	ASP	CA-CB-CG	6.02	118.62	112.60	9	1
L	19	PHE	N-CA-CB	6.01	100.29	110.50	9	1
G	11	GLU	C-N-CA	5.97	132.45	121.70	7	1
W	6	HIS	CB-CG-CD2	5.80	123.66	131.20	9	7
G	15	GLN	OE1-CD-NE2	5.79	116.81	122.60	8	2
K	19	PHE	CA-CB-CG	5.77	119.57	113.80	1	2
X	5	ARG	NE-CZ-NH1	5.73	127.23	121.50	9	1
V	41	ILE	CA-CB-CG1	5.73	120.14	110.40	5	1
J	38	GLY	C-N-CA	5.72	131.99	121.70	9	1
B	32	ILE	C-N-CA	5.71	131.99	121.70	9	1
G	13	HIS	CA-CB-CG	5.66	119.46	113.80	5	1
I	23	ASP	CA-CB-CG	5.65	118.25	112.60	5	6
J	13	HIS	CA-CB-CG	5.65	119.45	113.80	9	2
R	24	VAL	CA-CB-CG1	5.62	119.96	110.40	8	1
H	23	ASP	C-N-CA	5.60	131.78	121.70	9	1
B	27	ASN	OD1-CG-ND2	5.58	117.02	122.60	9	2
N	23	ASP	CA-CB-CG	5.56	118.16	112.60	9	7
F	37	GLY	C-N-CA	5.56	131.70	121.70	9	1
E	35	MET	C-N-CA	5.56	131.70	121.70	10	1
X	28	LYS	C-N-CA	5.52	131.64	121.70	9	1
E	15	GLN	OE1-CD-NE2	5.50	117.10	122.60	3	5
S	19	PHE	CA-CB-CG	5.50	119.30	113.80	2	1
J	42	ALA	C-CA-CB	5.45	118.67	110.50	9	1
O	18	VAL	N-CA-CB	5.42	102.29	111.50	10	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
I	13	HIS	CB-CG-CD2	5.42	124.16	131.20	1	6
L	21	ALA	N-CA-CB	5.41	102.29	110.40	9	1
H	24	VAL	CA-CB-CG1	5.40	119.59	110.40	9	2
J	6	HIS	CB-CG-CD2	5.40	124.19	131.20	1	8
P	3	GLU	N-CA-CB	5.39	101.33	110.50	9	1
H	23	ASP	CA-CB-CG	5.38	117.98	112.60	7	5
D	24	VAL	CA-C-N	5.36	126.93	116.20	9	1
P	16	LYS	CB-CG-CD	5.32	123.54	111.30	4	1
J	13	HIS	CB-CG-CD2	5.32	124.29	131.20	8	7
D	39	VAL	C-N-CA	5.31	131.26	121.70	9	1
D	19	PHE	CA-CB-CG	5.30	119.10	113.80	10	1
E	30	ALA	CA-C-O	5.29	111.80	120.80	10	1
M	19	PHE	CA-CB-CG	5.29	108.51	113.80	10	1
H	6	HIS	CB-CG-CD2	5.27	124.35	131.20	9	6
D	6	HIS	CB-CG-ND1	5.27	130.60	122.70	10	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	0.07	1
2	0.47	7
3	0.20	3
4	0.27	4
5	0.20	3
6	0.20	3
7	0.73	11
8	0.20	3
9	0.80	12
10	0.13	2

There are 49 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
L:22:GLU:OE2	R:22:GLU:N	0.96	7	1
L:22:GLU:OE1	R:24:VAL:HG22	0.90	7	1
V:14:HIS:CE1	V:17:LEU:HD13	0.83	9	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
V:14:HIS:CE1	X:14:HIS:CB	0.74	9	1
Q:35:MET:HB3	S:35:MET:SD	0.72	7	1
V:14:HIS:CE1	X:14:HIS:HB2	0.72	9	1
S:18:VAL:O	S:18:VAL:HG12	0.71	8	1
K:34:LEU:HD23	Q:34:LEU:HB3	0.71	2	1
L:22:GLU:OE2	R:21:ALA:C	0.70	7	1
G:22:GLU:O	G:23:ASP:OD1	0.69	5	1
L:22:GLU:OE1	R:24:VAL:HG13	0.68	7	1
L:22:GLU:OE1	R:24:VAL:CG2	0.65	7	1
V:34:LEU:HG	V:35:MET:HG2	0.62	3	1
J:36:VAL:O	J:36:VAL:HG12	0.61	9	1
S:32:ILE:CG2	S:35:MET:SD	0.59	7	1
K:34:LEU:CD2	Q:34:LEU:HB3	0.57	2	1
V:14:HIS:ND1	X:14:HIS:HB2	0.54	9	1
G:12:VAL:HG22	G:13:HIS:H	0.53	4	1
J:36:VAL:CG1	J:36:VAL:O	0.52	9	1
L:22:GLU:OE1	R:24:VAL:CG1	0.51	7	1
S:32:ILE:HG22	S:35:MET:SD	0.51	7	1
V:35:MET:SD	X:36:VAL:HB	0.49	3	1
V:14:HIS:CE1	X:14:HIS:CD2	0.49	9	1
P:6:HIS:CG	P:7:ASP:H	0.49	6	1
S:16:LYS:HE2	S:19:PHE:CD1	0.48	6	1
L:19:PHE:CD1	R:19:PHE:CE2	0.48	9	1
S:16:LYS:HE2	S:19:PHE:CG	0.47	5	2
V:14:HIS:CE1	X:14:HIS:CG	0.47	9	1
S:32:ILE:HG21	S:35:MET:HE2	0.46	7	1
G:5:ARG:HG3	G:36:VAL:HG12	0.46	8	1
K:17:LEU:CD1	K:34:LEU:HG	0.46	2	1
S:18:VAL:CG1	S:18:VAL:O	0.45	8	1
G:22:GLU:O	G:23:ASP:CG	0.43	5	1
K:17:LEU:CD1	K:34:LEU:CD2	0.43	2	1
K:17:LEU:HD13	K:34:LEU:CD2	0.43	2	1
W:28:LYS:HA	W:28:LYS:HE2	0.43	4	1
B:18:VAL:HG12	B:20:PHE:CE1	0.42	10	1
K:17:LEU:CD1	K:34:LEU:HD21	0.42	2	1
V:14:HIS:CE1	X:14:HIS:HB3	0.42	9	1
G:22:GLU:HG2	G:23:ASP:H	0.42	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
J:42:ALA:HB3	P:42:ALA:HA	0.42	9	1
S:32:ILE:CG2	S:35:MET:CG	0.42	7	1
U:19:PHE:CD1	W:16:LYS:HE2	0.41	4	1
V:14:HIS:ND1	X:14:HIS:CB	0.41	9	1
N:22:GLU:HG2	N:23:ASP:H	0.41	2	1
H:10:TYR:H	H:13:HIS:CE1	0.41	10	1
O:16:LYS:HE3	O:19:PHE:CE2	0.41	1	1
A:34:LEU:HB3	C:34:LEU:HD23	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	960	847	113	0
2	960	863	97	0
3	960	862	98	0
4	960	865	95	0
5	960	856	103	1
6	960	844	116	0
7	960	858	102	0
8	960	855	105	0
9	960	855	105	0
10	960	841	119	0

There are 1 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
O	9	GLY	1

### 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	768	737	27	4
2	768	740	24	4
3	768	737	27	4
4	768	731	28	9
5	768	736	28	4
6	768	742	25	1

Model ID	Analysed	Favored	Allowed	Outliers
7	768	753	15	0
8	768	757	11	0
9	768	728	31	9
10	768	714	41	13

*There are 43 unique sidechain outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
J	34	LEU	2
L	34	LEU	2
S	31	ILE	2
V	41	ILE	2
X	34	LEU	2
A	32	ILE	1
A	36	VAL	1
B	3	GLU	1
B	10	TYR	1
B	11	GLU	1
B	34	LEU	1
E	34	LEU	1
E	36	VAL	1
F	16	LYS	1
G	34	LEU	1
H	12	VAL	1
H	13	HIS	1
I	3	GLU	1
I	34	LEU	1
J	26	SER	1
K	34	LEU	1
L	5	ARG	1
L	11	GLU	1
M	3	GLU	1
M	16	LYS	1
M	41	ILE	1
N	3	GLU	1
N	16	LYS	1
O	5	ARG	1
O	10	TYR	1

Chain	Res	Type	Models (Total)
O	11	GLU	1
O	15	GLN	1
R	34	LEU	1
S	5	ARG	1
S	10	TYR	1
S	15	GLN	1
S	22	GLU	1
S	41	ILE	1
T	13	HIS	1
W	3	GLU	1
W	36	VAL	1
X	35	MET	1
X	41	ILE	1

### Fit of model to data used for modeling ?

#### 3DEM volume

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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