

Integrative Structure Validation Report ?

February 27, 2025 - 12:20 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	9A8E
PDB-Dev ID	PDBDEV_00000378
Structure Title	Type I 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

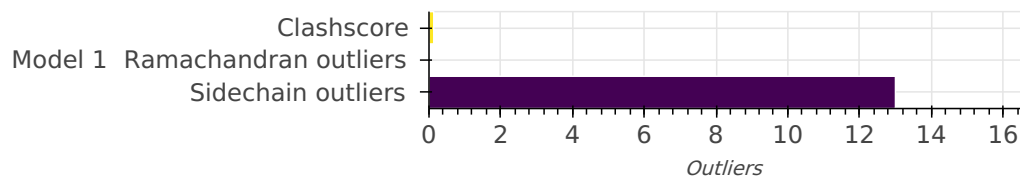
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

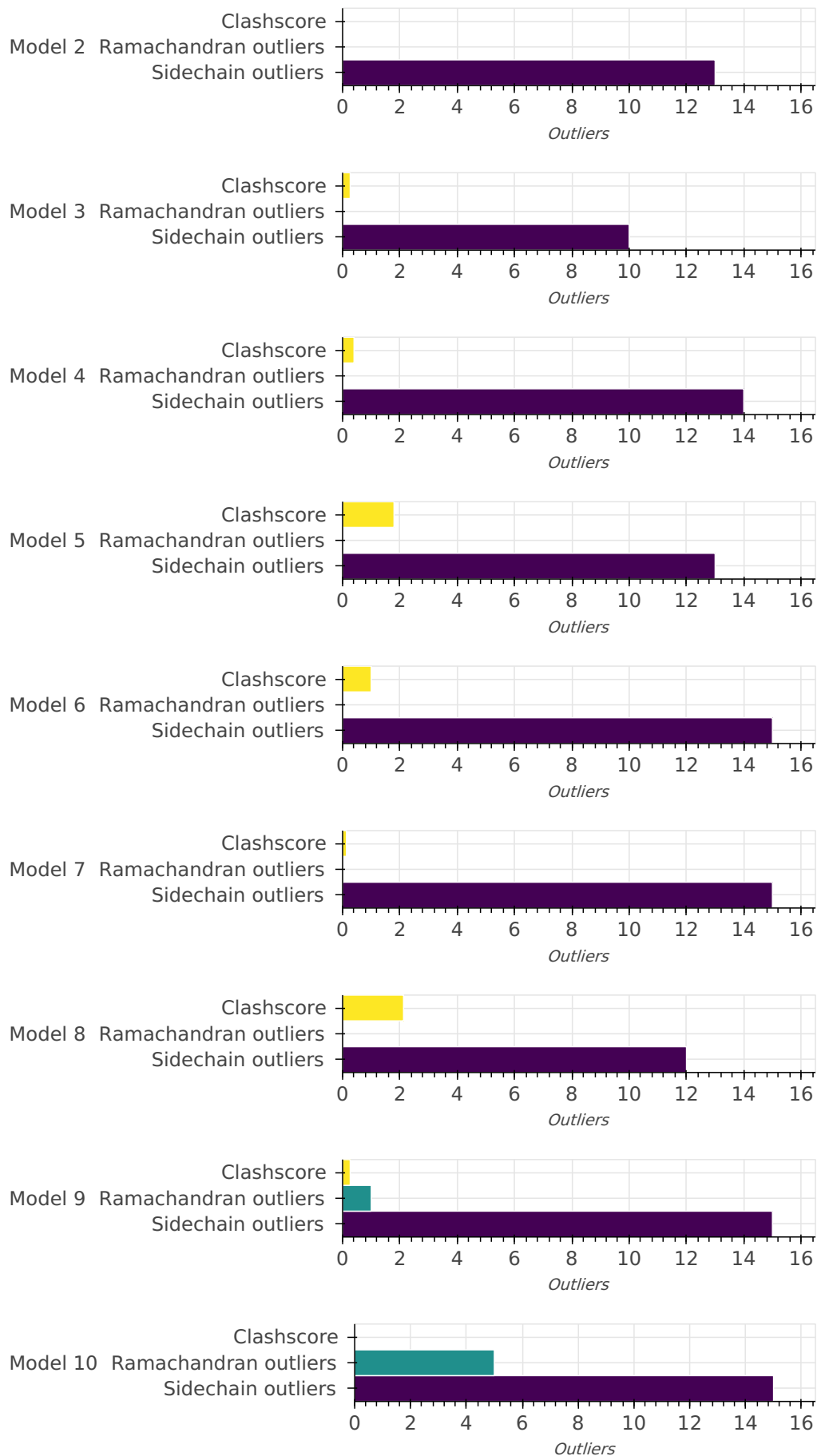
List of references used to build this report is available [here](#).

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 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	7q4b
5	3DEM volume	Zenodo	10.5281/zenodo.14766466
1	3DEM volume	EMDB	EMD-13800

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 https://zenodo.org/records/14766466 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	gmmconvert	Not available	express the experimental voxel map data as GMM data	https://gitlab.pasteur.fr/rpellari/recursive-gmconvert
2	Gromacs	GROMACS-2020.5	free and open-source software suite for high-performance molecular dynamics and output analysis	https://www.gromacs.org
3	Plumed	PLUMED.2.6.0-dev	enhanced-sampling algorithms	https://github.com/tlhr/plumed2.git

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 90 bond length outliers in this entry (0.12% of 78000 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	23	ASP	CG-OD2	28.01	0.72	1.25	7	1
A	23	ASP	CG-OD1	15.74	0.95	1.25	7	1
G	32	ILE	C-N	9.88	1.19	1.33	8	1
R	8	SER	C-O	9.43	1.04	1.23	8	1
G	32	ILE	C-O	9.39	1.04	1.23	8	1
R	8	SER	CB-OG	8.57	1.25	1.42	8	1
I	34	LEU	CG-CD1	8.39	1.24	1.52	8	1
W	19	PHE	CA-CB	8.31	1.70	1.53	5	1
A	14	HIS	ND1-CE1	8.09	1.40	1.32	8	1
I	34	LEU	CG-CD2	7.78	1.26	1.52	8	1
I	34	LEU	CB-CG	7.47	1.38	1.53	8	1
B	14	HIS	CE1-NE2	6.87	1.39	1.32	8	1
J	14	HIS	ND1-CE1	6.71	1.39	1.32	8	1
S	14	HIS	ND1-CE1	6.60	1.39	1.32	8	1
D	38	GLY	CA-C	6.22	1.63	1.52	5	1
O	14	HIS	CE1-NE2	6.15	1.38	1.32	8	1
O	31	ILE	N-CA	6.10	1.57	1.46	8	1
W	19	PHE	CB-CG	6.01	1.64	1.50	5	1
B	13	HIS	ND1-CE1	5.87	1.38	1.32	8	1
W	5	ARG	CZ-NH2	5.84	1.25	1.33	8	1
G	5	ARG	NE-CZ	5.74	1.26	1.33	5	1
I	20	PHE	N-CA	5.74	1.57	1.46	8	1
G	14	HIS	ND1-CE1	5.73	1.38	1.32	8	1
C	6	HIS	ND1-CE1	5.65	1.38	1.32	8	1
L	14	HIS	CB-CG	5.59	1.58	1.50	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
H	14	HIS	ND1-CE1	5.58	1.38	1.32	5	2
G	5	ARG	CZ-NH1	5.50	1.25	1.32	5	2
H	28	LYS	N-CA	5.43	1.56	1.46	8	1
D	18	VAL	N-CA	5.39	1.56	1.46	5	1
C	21	ALA	N-CA	5.35	1.36	1.46	8	1
P	23	ASP	C-N	5.22	1.40	1.33	8	1
D	28	LYS	CA-CB	5.10	1.63	1.53	8	1
L	14	HIS	CD2-NE2	5.01	1.32	1.37	8	1
A	22	GLU	C-N	5.00	1.40	1.33	8	1
N	5	ARG	CZ-NH2	4.99	1.27	1.33	4	1
D	14	HIS	CE1-NE2	4.98	1.37	1.32	8	1
I	15	GLN	CD-NE2	4.87	1.23	1.33	5	1
F	14	HIS	CG-ND1	4.84	1.43	1.38	8	1
J	19	PHE	CA-CB	4.80	1.43	1.53	5	1
G	6	HIS	ND1-CE1	4.76	1.37	1.32	8	1
S	13	HIS	ND1-CE1	4.73	1.37	1.32	8	1
L	28	LYS	C-N	4.73	1.40	1.33	8	1
L	23	ASP	CG-OD1	4.71	1.16	1.25	4	1
L	30	ALA	C-N	4.65	1.39	1.33	8	1
J	14	HIS	CD2-NE2	4.63	1.32	1.37	8	1
G	3	GLU	CA-CB	4.61	1.62	1.53	5	1
W	14	HIS	CB-CG	4.60	1.56	1.50	8	1
E	35	MET	SD-CE	4.59	1.91	1.79	8	1
J	5	ARG	CZ-NH1	4.56	1.26	1.32	5	1
B	14	HIS	CG-ND1	4.53	1.43	1.38	5	1
J	5	ARG	NE-CZ	4.52	1.28	1.33	8	1
H	13	HIS	CG-CD2	4.51	1.40	1.35	8	1
B	28	LYS	C-N	4.51	1.39	1.33	5	1
S	37	GLY	N-CA	4.49	1.52	1.45	5	1
D	10	TYR	CE2-CZ	4.48	1.49	1.38	8	1
K	35	MET	SD-CE	4.48	1.90	1.79	8	1
W	14	HIS	ND1-CE1	4.48	1.37	1.32	8	1
D	22	GLU	C-N	4.45	1.39	1.33	5	1
C	13	HIS	ND1-CE1	4.45	1.37	1.32	8	1
N	30	ALA	C-N	4.44	1.39	1.33	8	1
D	23	ASP	C-N	4.40	1.39	1.33	5	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	37	GLY	C-N	4.39	1.39	1.33	8	1
C	6	HIS	CE1-NE2	4.37	1.36	1.32	8	1
H	14	HIS	CD2-NE2	4.35	1.33	1.37	5	1
L	6	HIS	CG-ND1	4.34	1.43	1.38	5	1
B	13	HIS	CB-CG	4.34	1.56	1.50	8	1
S	13	HIS	CG-ND1	4.25	1.42	1.38	8	1
S	38	GLY	CA-C	4.22	1.59	1.52	5	1
B	14	HIS	CB-CG	4.22	1.56	1.50	5	1
C	14	HIS	ND1-CE1	4.20	1.36	1.32	8	1
J	5	ARG	CA-C	4.19	1.61	1.52	5	1
H	14	HIS	CE1-NE2	4.19	1.28	1.32	5	1
E	19	PHE	CG-CD1	4.17	1.47	1.38	8	1
G	14	HIS	CB-CG	4.17	1.44	1.50	8	1
L	32	ILE	CB-CG1	4.16	1.61	1.53	5	1
P	32	ILE	CB-CG1	4.13	1.45	1.53	8	1
Q	18	VAL	C-N	4.13	1.39	1.33	5	1
D	28	LYS	N-CA	4.11	1.54	1.46	8	1
E	40	VAL	CA-C	4.07	1.44	1.52	8	1
H	22	GLU	C-N	4.06	1.39	1.33	5	1
B	35	MET	CG-SD	4.03	1.70	1.80	5	1
M	35	MET	N-CA	4.03	1.53	1.46	8	1
N	40	VAL	N-CA	4.03	1.53	1.46	5	1
W	19	PHE	N-CA	4.02	1.53	1.46	5	1
K	21	ALA	C-N	4.01	1.27	1.33	8	1
H	13	HIS	C-N	4.01	1.39	1.33	8	1
P	37	GLY	C-N	4.01	1.27	1.33	8	1
N	5	ARG	CZ-NH1	4.00	1.27	1.32	4	1

Standard geometry: angle outliers ?

There are 846 bond angle outliers in this entry (0.81% 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)
A	23	ASP	OD1-CG-OD2	13.75	89.91	122.90	7	1
A	23	ASP	CB-CG-OD1	13.36	149.14	118.40	7	1
S	15	GLN	OE1-CD-NE2	11.30	111.30	122.60	8	4
W	19	PHE	CA-CB-CG	10.43	124.23	113.80	5	1
D	15	GLN	OE1-CD-NE2	9.11	113.49	122.60	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
H	7	ASP	CA-CB-CG	9.11	121.71	112.60	3	2
D	14	HIS	CB-CG-CD2	9.02	119.47	131.20	5	4
W	19	PHE	N-CA-CB	8.64	125.19	110.50	5	1
U	19	PHE	CB-CG-CD1	8.55	106.16	120.70	5	1
N	27	ASN	OD1-CG-ND2	8.48	114.12	122.60	8	1
C	23	ASP	CA-CB-CG	8.45	121.05	112.60	8	2
J	4	PHE	CA-CB-CG	8.39	122.19	113.80	8	1
A	23	ASP	CA-CB-CG	8.34	120.94	112.60	8	5
I	34	LEU	CD1-CG-CD2	8.30	92.54	110.80	8	1
S	15	GLN	CG-CD-NE2	8.29	128.83	116.40	8	1
E	23	ASP	CA-CB-CG	8.16	120.76	112.60	7	2
P	14	HIS	CB-CG-CD2	8.10	120.67	131.20	8	2
C	27	ASN	CA-CB-CG	7.84	104.76	112.60	8	1
D	42	ALA	C-CA-CB	7.75	122.13	110.50	5	1
G	32	ILE	O-C-N	7.63	110.80	123.00	8	1
L	6	HIS	ND1-CE1-NE2	7.39	115.79	108.40	5	1
K	23	ASP	CA-CB-CG	7.33	119.93	112.60	10	2
D	22	GLU	CA-CB-CG	7.32	128.73	114.10	8	1
U	19	PHE	CA-CB-CG	7.26	121.06	113.80	10	2
K	14	HIS	CA-CB-CG	7.10	120.90	113.80	8	1
S	14	HIS	C-CA-CB	7.05	123.49	110.10	8	1
E	4	PHE	CA-CB-CG	6.95	120.75	113.80	5	2
J	27	ASN	C-N-CA	6.93	134.17	121.70	8	1
L	27	ASN	OD1-CG-ND2	6.91	115.69	122.60	8	1
U	19	PHE	CB-CG-CD2	6.83	132.32	120.70	5	1
O	14	HIS	CB-CG-CD2	6.83	122.33	131.20	8	4
D	27	ASN	OD1-CG-ND2	6.79	115.81	122.60	8	3
J	27	ASN	OD1-CG-ND2	6.73	115.87	122.60	5	2
C	24	VAL	CA-CB-CG2	6.64	121.70	110.40	8	1
S	14	HIS	CA-CB-CG	6.63	120.43	113.80	8	1
D	28	LYS	CA-CB-CG	6.61	100.89	114.10	8	1
D	23	ASP	CA-CB-CG	6.60	119.20	112.60	2	3
A	27	ASN	OD1-CG-ND2	6.55	116.05	122.60	8	1
H	27	ASN	CA-CB-CG	6.54	106.06	112.60	8	1
W	19	PHE	CB-CG-CD2	6.49	131.74	120.70	5	1
J	24	VAL	CA-CB-CG2	6.45	121.37	110.40	8	1
D	14	HIS	ND1-CG-CD2	6.45	112.55	106.10	5	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
J	23	ASP	CA-CB-CG	6.42	119.02	112.60	10	3
P	14	HIS	ND1-CG-CD2	6.40	112.50	106.10	8	1
W	4	PHE	CA-CB-CG	6.39	120.19	113.80	1	2
I	1	ASP	CA-CB-CG	6.36	118.96	112.60	5	1
N	23	ASP	CA-CB-CG	6.31	118.91	112.60	6	2
O	36	VAL	CA-CB-CG1	6.28	121.08	110.40	8	1
K	19	PHE	C-N-CA	6.28	133.00	121.70	8	1
H	27	ASN	OD1-CG-ND2	6.27	116.33	122.60	5	2
H	27	ASN	C-CA-CB	6.20	121.89	110.10	5	1
G	6	HIS	ND1-CE1-NE2	6.20	114.60	108.40	8	1
X	13	HIS	CA-CB-CG	6.17	119.97	113.80	9	2
O	13	HIS	CA-CB-CG	6.12	119.92	113.80	10	3
B	2	ALA	C-CA-CB	6.11	119.66	110.50	8	1
K	14	HIS	CB-CG-CD2	6.09	123.28	131.20	8	4
U	19	PHE	CD1-CE1-CZ	6.07	130.92	120.00	5	1
H	27	ASN	C-N-CA	6.05	132.58	121.70	5	1
B	6	HIS	ND1-CE1-NE2	6.02	114.42	108.40	8	1
O	20	PHE	CA-CB-CG	6.02	119.82	113.80	8	2
G	6	HIS	CB-CG-CD2	6.00	123.40	131.20	8	6
J	28	LYS	CA-C-O	5.97	110.65	120.80	5	1
W	7	ASP	CA-CB-CG	5.95	118.55	112.60	1	3
G	3	GLU	C-N-CA	5.95	132.41	121.70	5	1
R	8	SER	CA-CB-OG	5.93	122.97	111.10	8	1
I	15	GLN	CB-CG-CD	5.92	122.67	112.60	5	1
P	23	ASP	CA-CB-CG	5.90	118.50	112.60	6	3
A	37	GLY	CA-C-N	5.90	127.99	116.20	8	1
P	27	ASN	OD1-CG-ND2	5.86	116.74	122.60	8	1
E	3	GLU	C-CA-CB	5.85	98.98	110.10	5	1
B	2	ALA	C-N-CA	5.79	132.13	121.70	8	1
L	21	ALA	C-N-CA	5.79	132.12	121.70	8	1
D	27	ASN	CA-CB-CG	5.79	106.81	112.60	8	1
O	24	VAL	C-N-CA	5.77	132.08	121.70	8	1
K	18	VAL	CA-CB-CG2	5.76	120.19	110.40	8	1
V	19	PHE	CA-CB-CG	5.75	119.55	113.80	8	2
H	21	ALA	C-CA-CB	5.72	119.08	110.50	5	1
K	14	HIS	C-CA-CB	5.71	120.96	110.10	8	1
C	18	VAL	CG1-CB-CG2	5.71	98.25	110.80	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	32	ILE	CA-CB-CG2	5.68	120.15	110.50	5	1
L	6	HIS	N-CA-CB	5.65	100.89	110.50	5	1
R	6	HIS	CA-CB-CG	5.65	119.45	113.80	2	1
L	23	ASP	CA-CB-CG	5.64	118.24	112.60	4	3
H	6	HIS	C-N-CA	5.61	131.79	121.70	3	1
B	6	HIS	CA-CB-CG	5.60	119.40	113.80	8	1
W	18	VAL	C-N-CA	5.59	131.77	121.70	5	1
A	22	GLU	O-C-N	5.57	114.09	123.00	8	1
J	7	ASP	CA-CB-CG	5.56	118.16	112.60	10	2
U	15	GLN	OE1-CD-NE2	5.55	117.05	122.60	1	4
H	23	ASP	CA-CB-CG	5.54	118.14	112.60	4	3
S	7	ASP	CA-CB-CG	5.52	118.12	112.60	5	1
D	7	ASP	CA-CB-CG	5.51	118.11	112.60	10	1
P	31	ILE	CA-C-O	5.49	111.47	120.80	8	1
M	35	MET	N-CA-CB	5.47	101.20	110.50	8	1
D	21	ALA	C-CA-CB	5.46	118.69	110.50	5	1
U	13	HIS	CA-CB-CG	5.43	119.23	113.80	3	3
M	32	ILE	CA-CB-CG2	5.41	119.70	110.50	5	1
N	42	ALA	N-CA-CB	5.40	102.31	110.40	8	1
T	13	HIS	CB-CG-CD2	5.39	124.19	131.20	6	7
H	12	VAL	CA-CB-CG2	5.39	119.56	110.40	8	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	0.13	2
2	0.00	0
3	0.27	4
4	0.40	6
5	1.79	27
6	1.00	15
7	0.13	2
8	2.13	32
9	0.27	4
10	0.00	0

There are 92 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)
N:24:VAL:CG1	N:27:ASN:HD21	1.55	8	1
N:24:VAL:HG12	N:27:ASN:ND2	1.36	8	1
N:24:VAL:CG1	N:27:ASN:ND2	1.22	8	1
N:24:VAL:HG11	N:27:ASN:HD21	1.07	8	1
E:19:PHE:CZ	E:34:LEU:HD21	1.04	8	1
E:19:PHE:HZ	E:34:LEU:HD21	0.97	8	1
A:34:LEU:HD13	E:34:LEU:HD22	0.96	8	1
N:24:VAL:HG12	N:27:ASN:HD21	0.95	8	1
L:31:ILE:HD11	N:27:ASN:HD22	0.87	8	1
A:34:LEU:HB3	E:34:LEU:HD23	0.85	8	1
U:19:PHE:HE1	W:19:PHE:H	0.85	5	1
E:19:PHE:CZ	E:34:LEU:CD2	0.85	8	1
U:19:PHE:HE1	W:19:PHE:N	0.79	5	1
U:19:PHE:CE1	W:19:PHE:CD2	0.75	5	1
A:34:LEU:HD13	E:34:LEU:CD2	0.74	8	1
E:19:PHE:CE2	E:34:LEU:CD2	0.72	8	1
D:22:GLU:HB3	H:23:ASP:OD1	0.70	5	1
L:31:ILE:CD1	N:27:ASN:HD22	0.69	8	1
U:19:PHE:CZ	W:19:PHE:CD2	0.69	5	1
I:22:GLU:HB3	O:23:ASP:OD1	0.68	4	1
U:17:LEU:HD13	U:19:PHE:CE2	0.66	5	1
S:12:VAL:O	S:12:VAL:HG12	0.66	9	1
A:22:GLU:HB3	C:23:ASP:OD1	0.65	4	2
U:17:LEU:HD13	U:19:PHE:HE2	0.64	5	1
D:24:VAL:CG1	D:27:ASN:ND2	0.64	6	1
E:19:PHE:CE2	E:34:LEU:HD21	0.64	8	1
B:23:ASP:OD1	D:23:ASP:CG	0.64	3	1
E:19:PHE:CZ	E:34:LEU:CG	0.63	8	1
D:23:ASP:OD1	H:23:ASP:CG	0.63	5	1
U:19:PHE:CE1	W:19:PHE:N	0.63	5	1
B:23:ASP:OD1	D:23:ASP:OD1	0.63	3	1
I:23:ASP:N	O:23:ASP:OD1	0.61	4	1
Q:11:GLU:HB3	S:12:VAL:HG11	0.61	9	1
D:27:ASN:OD1	H:27:ASN:HB2	0.60	6	1
D:23:ASP:OD1	H:23:ASP:OD1	0.60	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
D:24:VAL:HG12	D:27:ASN:HD22	0.60	6	1
L:24:VAL:HG12	L:27:ASN:ND2	0.60	8	1
D:24:VAL:CG1	D:27:ASN:HD22	0.59	6	1
L:20:PHE:CD2	P:20:PHE:CE1	0.59	8	1
D:24:VAL:HG13	D:27:ASN:ND2	0.57	6	1
B:22:GLU:HB3	D:23:ASP:OD1	0.56	3	1
E:19:PHE:CZ	E:34:LEU:HG	0.55	8	1
L:17:LEU:C	L:17:LEU:HD23	0.54	8	1
D:27:ASN:ND2	D:31:ILE:CD1	0.54	6	1
A:34:LEU:HB3	E:34:LEU:CD2	0.54	8	1
D:27:ASN:ND2	D:31:ILE:HD11	0.53	6	1
N:24:VAL:HG11	N:27:ASN:ND2	0.53	8	1
C:22:GLU:HG3	C:23:ASP:H	0.52	5	1
S:12:VAL:CG1	S:12:VAL:O	0.52	9	1
L:24:VAL:HG12	L:27:ASN:HD22	0.51	8	1
C:1:ASP:H1	F:42:ALA:C	0.51	9	1
L:24:VAL:CG1	L:27:ASN:ND2	0.51	8	1
H:22:GLU:HB3	J:23:ASP:OD1	0.51	7	1
L:27:ASN:CG	L:31:ILE:HD11	0.51	8	1
L:21:ALA:HA	P:21:ALA:HB3	0.51	5	1
U:19:PHE:CD1	W:19:PHE:CD2	0.51	5	1
R:35:MET:HE2	R:37:GLY:O	0.50	1	1
L:27:ASN:ND2	L:31:ILE:CD1	0.50	8	1
D:24:VAL:HG13	D:27:ASN:HD21	0.49	6	1
U:19:PHE:CE1	W:19:PHE:CG	0.49	5	1
A:34:LEU:CD1	E:34:LEU:CD2	0.49	8	1
D:23:ASP:CG	H:23:ASP:CG	0.49	5	1
D:23:ASP:N	H:23:ASP:OD1	0.48	5	1
E:19:PHE:CE2	E:34:LEU:HD23	0.48	8	1
U:18:VAL:O	U:19:PHE:CE1	0.48	5	1
D:24:VAL:HG12	D:27:ASN:ND2	0.47	6	1
C:18:VAL:HG11	C:21:ALA:HB2	0.47	8	1
U:19:PHE:CE1	W:19:PHE:CB	0.47	5	1
D:23:ASP:OD1	H:23:ASP:OD2	0.47	5	1
C:23:ASP:HB2	G:23:ASP:OD1	0.46	1	1
U:19:PHE:HE1	W:19:PHE:CA	0.46	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
N:27:ASN:ND2	N:31:ILE:HG13	0.46	8	1
B:23:ASP:OD1	F:22:GLU:HB3	0.46	4	1
J:27:ASN:ND2	J:31:ILE:CD1	0.45	6	1
J:24:VAL:O	J:27:ASN:ND2	0.45	6	1
J:27:ASN:ND2	J:31:ILE:HD11	0.45	6	1
J:27:ASN:OD1	P:27:ASN:N	0.45	6	1
N:24:VAL:HG12	N:27:ASN:CG	0.45	8	1
I:3:GLU:CD	I:3:GLU:H	0.43	5	1
B:23:ASP:N	D:23:ASP:OD1	0.43	3	1
T:41:ILE:H	T:41:ILE:HD13	0.42	7	1
M:1:ASP:HA	M:6:HIS:CE1	0.42	6	1
L:27:ASN:ND2	L:31:ILE:HD12	0.42	8	1
G:15:GLN:HE21	I:15:GLN:HG2	0.41	5	1
M:19:PHE:CE2	Q:19:PHE:CE2	0.41	5	1
N:6:HIS:CG	N:7:ASP:H	0.41	5	1
G:22:GLU:HG2	G:23:ASP:H	0.41	5	1
N:34:LEU:HD11	N:36:VAL:CG2	0.41	5	1
A:23:ASP:N	C:23:ASP:OD1	0.41	4	1
H:17:LEU:HD23	H:18:VAL:N	0.41	5	1
A:22:GLU:CB	C:23:ASP:OD1	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	880	80	0
2	960	862	98	0
3	960	870	90	0
4	960	878	82	0
5	960	854	106	0
6	960	876	84	0
7	960	861	99	0
8	960	860	100	0
9	960	877	82	1
10	960	877	78	5

There are 5 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
S	12	VAL	2
N	24	VAL	1
T	33	GLY	1
T	41	ILE	1
V	12	VAL	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	702	53	13
2	768	720	35	13
3	768	722	36	10
4	768	717	37	14
5	768	701	54	13
6	768	711	42	15
7	768	713	40	15
8	768	707	49	12
9	768	711	42	15
10	768	711	42	15

There are 96 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
L	23	ASP	4
N	23	ASP	4
B	34	LEU	3
J	23	ASP	3
K	34	LEU	3
M	34	LEU	3
O	23	ASP	3
P	34	LEU	3
S	41	ILE	3
A	15	GLN	2
A	23	ASP	2
C	15	GLN	2
H	14	HIS	2
H	15	GLN	2
I	15	GLN	2

Chain	Res	Type	Models (Total)
I	23	ASP	2
I	34	LEU	2
M	6	HIS	2
O	34	LEU	2
P	23	ASP	2
Q	32	ILE	2
S	14	HIS	2
S	24	VAL	2
T	27	ASN	2
V	15	GLN	2
W	4	PHE	2
W	10	TYR	2
W	15	GLN	2
A	3	GLU	1
A	14	HIS	1
A	24	VAL	1
A	34	LEU	1
B	27	ASN	1
B	41	ILE	1
C	23	ASP	1
C	28	LYS	1
D	1	ASP	1
D	34	LEU	1
E	1	ASP	1
E	23	ASP	1
F	24	VAL	1
F	34	LEU	1
G	1	ASP	1
G	23	ASP	1
G	27	ASN	1
H	3	GLU	1
H	7	ASP	1
H	24	VAL	1
H	34	LEU	1
I	3	GLU	1
J	15	GLN	1

Chain	Res	Type	Models (Total)
J	27	ASN	1
J	34	LEU	1
K	3	GLU	1
K	11	GLU	1
K	14	HIS	1
K	23	ASP	1
L	3	GLU	1
L	7	ASP	1
L	22	GLU	1
M	17	LEU	1
N	22	GLU	1
N	24	VAL	1
N	34	LEU	1
O	7	ASP	1
O	22	GLU	1
P	28	LYS	1
Q	1	ASP	1
Q	17	LEU	1
Q	28	LYS	1
R	3	GLU	1
R	12	VAL	1
R	27	ASN	1
S	3	GLU	1
S	11	GLU	1
S	16	LYS	1
S	28	LYS	1
S	35	MET	1
T	1	ASP	1
T	13	HIS	1
T	41	ILE	1
U	5	ARG	1
U	15	GLN	1
U	19	PHE	1
U	20	PHE	1
U	31	ILE	1
V	6	HIS	1
V	11	GLU	1

Chain	Res	Type	Models (Total)
V	17	LEU	1
V	24	VAL	1
V	36	VAL	1
W	28	LYS	1
W	34	LEU	1
X	5	ARG	1
X	23	ASP	1
X	27	ASN	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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