

Integrative Structure Validation Report ?

March 27, 2025 - 10:09 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

PyMOL Version 2.5.0

PDB ID	9A1S
PDB-Dev ID	PDBDEV_00000112
Structure Title	Molten Globule Ensemble from Helicobacter pylori Flavodoxin
Structure Authors	Galano-Frutos JJ; Torreblanca R; Garcia-Cebollada H; Sancho J
Deposited on	2022-04-12

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

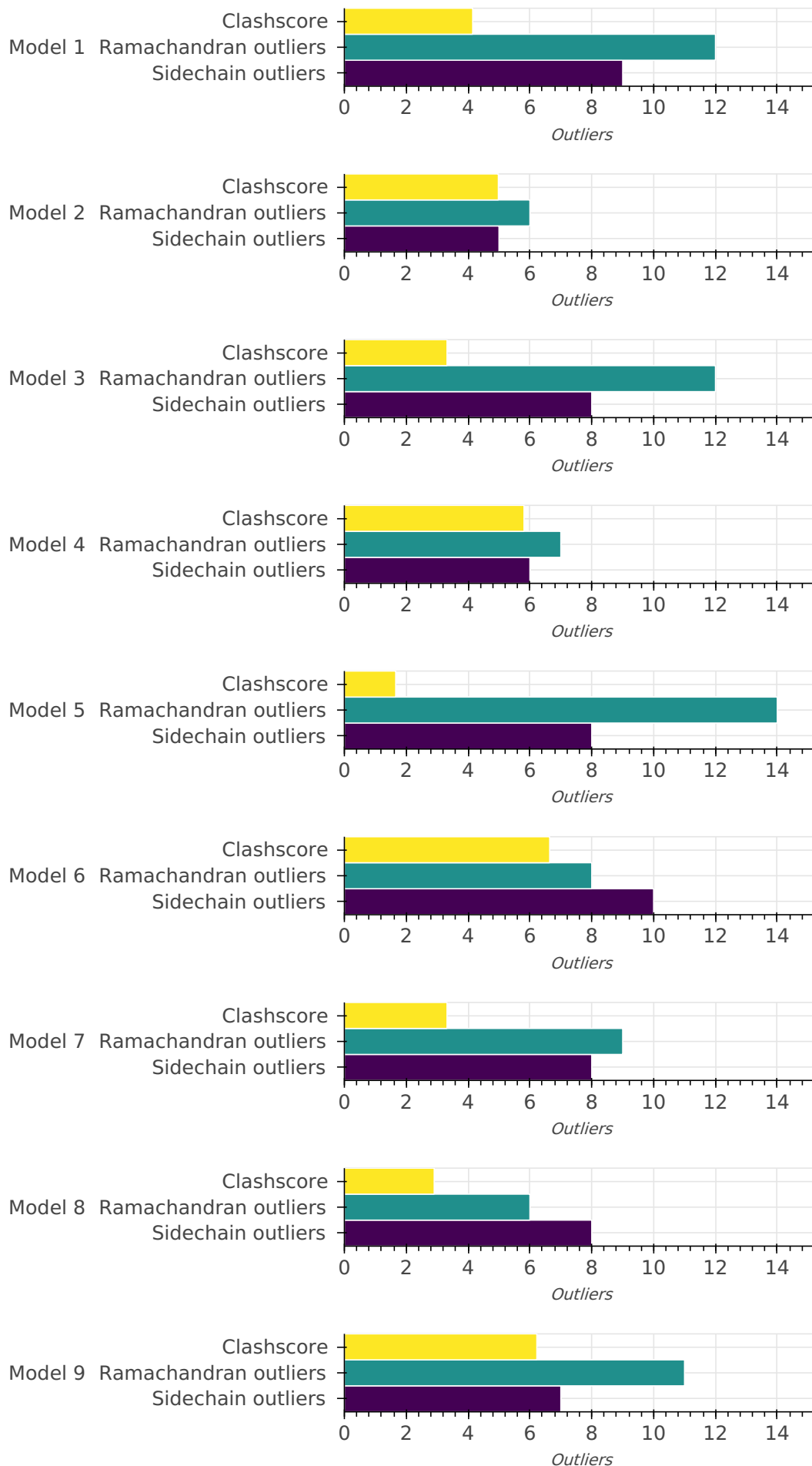
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

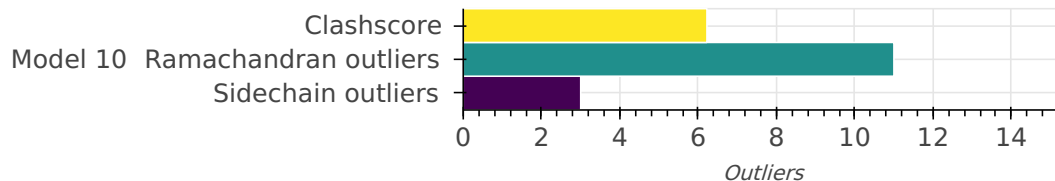
List of references used to build this report is available [here](#).

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 1 distinct ensemble(s).

Summary ?

This entry consists of 10 model(s). A total of 4 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	MOLTEN GLOBULE OF APOFLAVODOXIN FROM HELICOBACTER PYLORI, ELECTRON TRANSPORT	A	163	-	1-163	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	2BMV
2	Mutagenesis data	Not available	Not available
3	Other	Not available	Not available

ID	Dataset type	Database name	Data access code
4	Other	Not available	Not available

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	Generation of the initial ensemble	Biased (experimental phi-values) molecular dynamics simulations	Experimental phi-values from mutagenesis experiments are used as a reaction coordinate to bias a starting model using molecular dynamics simulations (HQB module from Charmm program)	21	False	False
2	1	Ensemble refinement	Ensemble refinement based on experimental spectroscopic data	A variety of spectroscopic data (fluorescence, far- and near-UV, and NMR) used for refining the initial biased MD ensemble	10	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	CHARMM	v.44b2	Molecular dynamics simulations	https://www.charmm.org/

Data quality ?

Mutagenesis

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 404 bond length outliers in this entry (3.24% of 12480 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	101	HIS	CD2-NE2	13.00	1.23	1.37	2	9
A	104	GLU	CD-OE1	12.81	1.44	1.19	8	5
A	74	ASP	CG-OD1	12.17	1.43	1.19	8	6
A	97	GLU	CD-OE1	11.85	1.42	1.19	1	6
A	118	ASP	CG-OD1	11.81	1.42	1.19	6	4
A	87	ASP	CG-OD1	11.80	1.42	1.19	3	2
A	15	GLU	CD-OE1	11.74	1.42	1.19	1	5
A	139	ASP	CG-OD1	11.66	1.42	1.19	4	2
A	10	ASP	CG-OD1	11.65	1.42	1.19	6	6
A	64	GLU	CD-OE1	11.65	1.42	1.19	7	5
A	129	GLU	CD-OE1	11.61	1.42	1.19	10	5
A	93	GLU	CD-OE1	11.48	1.41	1.19	7	3
A	19	GLU	CD-OE1	11.43	1.41	1.19	5	8
A	71	GLU	CD-OE1	11.36	1.41	1.19	6	6
A	123	GLU	CD-OE1	11.31	1.41	1.19	3	4
A	140	GLU	CD-OE1	11.03	1.41	1.19	2	8
A	156	GLU	CD-OE1	10.92	1.40	1.19	5	6
A	65	ASP	CG-OD1	10.80	1.40	1.19	2	4
A	141	ASP	CG-OD1	10.64	1.40	1.19	7	3
A	148	ASP	CG-OD1	10.57	1.40	1.19	3	2
A	39	GLU	CD-OE1	10.54	1.40	1.19	10	4
A	149	GLU	CD-OE1	10.49	1.39	1.19	7	2
A	29	GLU	CD-OE1	10.42	1.39	1.19	4	4
A	145	ASP	CG-OD1	10.22	1.39	1.19	8	4
A	32	ASP	CG-OD1	10.07	1.39	1.19	1	5
A	62	ASP	CG-OD1	9.96	1.38	1.19	9	5
A	89	ASP	CG-OD1	9.84	1.38	1.19	5	5
A	58	ASP	CG-OD1	9.84	1.38	1.19	5	2
A	144	ASP	CG-OD1	9.83	1.38	1.19	5	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	121	HIS	CD2-NE2	9.09	1.27	1.37	5	8
A	101	HIS	CG-ND1	8.41	1.29	1.38	3	6
A	93	GLU	CD-OE2	8.19	1.17	1.33	4	4
A	71	GLU	CD-OE2	8.01	1.17	1.33	1	5
A	121	HIS	CG-ND1	8.00	1.29	1.38	7	7
A	62	ASP	CG-OD2	7.61	1.18	1.33	9	3
A	104	GLU	CD-OE2	7.52	1.18	1.33	3	5
A	65	ASP	CG-OD2	7.44	1.18	1.33	4	4
A	121	HIS	CG-CD2	7.32	1.43	1.35	8	2
A	123	GLU	CD-OE2	7.27	1.18	1.33	1	4
A	89	ASP	CG-OD2	7.03	1.19	1.33	7	6
A	39	GLU	CD-OE2	6.99	1.19	1.33	4	3
A	39	GLU	C-N	6.97	1.43	1.33	4	1
A	156	GLU	CD-OE2	6.85	1.19	1.33	8	6
A	19	GLU	CD-OE2	6.73	1.20	1.33	8	6
A	32	ASP	CG-OD2	6.73	1.20	1.33	1	6
A	27	ASN	CA-CB	6.65	1.66	1.53	4	2
A	139	ASP	CG-OD2	6.61	1.20	1.33	9	2
A	101	HIS	CG-CD2	6.36	1.42	1.35	2	3
A	121	HIS	CB-CG	6.36	1.59	1.50	5	3
A	74	ASP	CG-OD2	6.31	1.20	1.33	5	6
A	154	TRP	NE1-CE2	6.31	1.30	1.37	8	2
A	144	ASP	CG-OD2	6.30	1.20	1.33	7	3
A	141	ASP	CG-OD2	6.29	1.46	1.33	8	3
A	154	TRP	CG-CD2	6.24	1.32	1.43	7	1
A	80	ILE	C-N	6.22	1.42	1.33	2	1
A	118	ASP	CG-OD2	6.20	1.21	1.33	3	3
A	10	ASP	CG-OD2	6.15	1.21	1.33	7	5
A	140	GLU	CD-OE2	6.12	1.21	1.33	1	9
A	145	ASP	CG-OD2	5.97	1.21	1.33	2	2
A	121	HIS	ND1-CE1	5.93	1.26	1.32	9	1
A	101	HIS	CB-CG	5.92	1.58	1.50	1	3
A	63	TRP	NE1-CE2	5.92	1.30	1.37	4	4
A	15	GLU	CD-OE2	5.90	1.21	1.33	10	3
A	148	ASP	CG-OD2	5.90	1.21	1.33	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	101	HIS	CE1-NE2	5.82	1.26	1.32	6	2
A	101	HIS	C-N	5.75	1.41	1.33	6	1
A	63	TRP	CD2-CE3	5.67	1.31	1.40	1	1
A	58	ASP	CG-OD2	5.61	1.44	1.33	4	3
A	129	GLU	CD-OE2	5.54	1.22	1.33	10	2
A	42	ASN	CA-CB	5.53	1.64	1.53	8	1
A	103	TYR	CA-CB	5.44	1.42	1.53	3	1
A	106	ALA	N-CA	5.43	1.35	1.46	9	1
A	101	HIS	CA-CB	5.41	1.64	1.53	4	1
A	59	LEU	CA-CB	5.39	1.64	1.53	7	1
A	154	TRP	CD2-CE3	5.36	1.31	1.40	8	2
A	121	HIS	CE1-NE2	5.31	1.27	1.32	1	2
A	89	ASP	C-N	5.23	1.40	1.33	1	2
A	160	GLY	N-CA	5.19	1.37	1.45	3	1
A	136	LEU	C-N	5.19	1.40	1.33	6	1
A	162	PHE	CB-CG	5.18	1.62	1.50	8	1
A	64	GLU	CD-OE2	5.14	1.23	1.33	9	4
A	29	GLU	CD-OE2	5.14	1.23	1.33	4	3
A	71	GLU	CA-CB	5.12	1.63	1.53	3	1
A	74	ASP	C-N	5.12	1.40	1.33	2	2
A	92	SER	C-N	5.09	1.40	1.33	8	1
A	87	ASP	CG-OD2	5.08	1.43	1.33	7	2
A	105	LYS	C-N	5.04	1.40	1.33	3	1
A	63	TRP	CG-CD2	5.00	1.34	1.43	3	1
A	154	TRP	CD2-CE2	4.99	1.32	1.41	9	1
A	97	GLU	CA-CB	4.96	1.43	1.53	2	1
A	155	VAL	C-N	4.94	1.40	1.33	6	1
A	52	PRO	N-CD	4.92	1.40	1.47	9	1
A	97	GLU	CD-OE2	4.91	1.23	1.33	1	3
A	133	PHE	C-N	4.90	1.26	1.33	6	1
A	120	TYR	C-N	4.85	1.40	1.33	4	1
A	32	ASP	CA-CB	4.81	1.63	1.53	6	1
A	150	ARG	CZ-NH1	4.80	1.39	1.32	6	1
A	77	ASN	C-N	4.79	1.40	1.33	1	2
A	98	GLY	CA-C	4.78	1.60	1.52	2	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	128	VAL	C-N	4.77	1.40	1.33	1	1

Standard geometry: angle outliers ?

There are 1004 bond angle outliers in this entry (5.96% of 16840 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	100	PHE	CA-CB-CG	10.82	124.62	113.80	6	6
A	42	ASN	OD1-CG-ND2	10.79	111.81	122.60	5	4
A	143	GLN	OE1-CD-NE2	10.67	111.93	122.60	5	6
A	13	ASN	OD1-CG-ND2	10.19	112.41	122.60	7	4
A	121	HIS	CB-CG-CD2	10.01	118.18	131.20	7	6
A	118	ASP	CA-CB-CG	9.92	122.52	112.60	8	3
A	101	HIS	CB-CG-CD2	9.83	118.42	131.20	10	5
A	101	HIS	CA-CB-CG	9.81	123.61	113.80	8	3
A	13	ASN	CA-CB-CG	9.77	122.37	112.60	4	4
A	63	TRP	NE1-CE2-CZ2	9.67	115.60	130.10	9	7
A	89	ASP	CA-CB-CG	9.56	122.16	112.60	6	5
A	121	HIS	CB-CG-ND1	9.44	136.85	122.70	7	5
A	88	GLN	OE1-CD-NE2	9.39	113.21	122.60	7	3
A	60	GLN	OE1-CD-NE2	9.35	113.25	122.60	9	6
A	139	ASP	CA-CB-CG	9.12	121.72	112.60	9	3
A	77	ASN	CB-CG-ND2	9.02	129.94	116.40	9	4
A	101	HIS	CB-CG-ND1	8.97	136.15	122.70	9	5
A	114	GLN	OE1-CD-NE2	8.89	113.71	122.60	3	3
A	142	ASN	CA-CB-CG	8.88	121.48	112.60	1	3
A	101	HIS	ND1-CG-CD2	8.87	114.97	106.10	8	1
A	114	GLN	CG-CD-NE2	8.85	129.67	116.40	3	1
A	32	ASP	CA-CB-CG	8.70	121.30	112.60	4	4
A	77	ASN	OD1-CG-ND2	8.65	113.95	122.60	9	9
A	16	ALA	N-CA-CB	8.65	97.43	110.40	6	4
A	27	ASN	OD1-CG-ND2	8.59	114.01	122.60	1	5
A	142	ASN	OD1-CG-ND2	8.59	114.01	122.60	6	3
A	45	THR	CA-CB-CG2	8.57	125.07	110.50	9	3
A	27	ASN	CA-CB-CG	8.56	121.16	112.60	9	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	42	ASN	CA-CB-CG	8.32	120.92	112.60	8	6
A	63	TRP	CD2-CE2-NE1	8.25	118.12	107.40	5	6
A	41	PHE	CA-CB-CG	8.17	121.97	113.80	2	2
A	154	TRP	CE2-CD2-CE3	8.07	126.87	118.80	9	4
A	63	TRP	CG-CD2-CE2	8.02	97.58	107.20	5	7
A	144	ASP	CA-CB-CG	7.96	120.56	112.60	2	4
A	28	ALA	C-CA-CB	7.95	98.58	110.50	8	2
A	133	PHE	CA-CB-CG	7.94	121.74	113.80	9	5
A	6	PHE	CA-CB-CG	7.80	121.60	113.80	1	5
A	40	GLN	OE1-CD-NE2	7.79	114.81	122.60	3	6
A	10	ASP	CA-CB-CG	7.73	120.33	112.60	5	4
A	75	PHE	CA-CB-CG	7.73	121.53	113.80	9	6
A	62	ASP	CA-CB-CG	7.72	120.32	112.60	10	4
A	154	TRP	NE1-CE2-CZ2	7.72	118.53	130.10	5	9
A	156	GLU	CA-CB-CG	7.67	129.43	114.10	7	1
A	162	PHE	CA-CB-CG	7.61	121.41	113.80	3	4
A	154	TRP	CG-CD1-NE1	7.57	100.35	110.20	8	3
A	77	ASN	CA-CB-CG	7.56	120.16	112.60	2	3
A	154	TRP	CD2-CE2-NE1	7.46	117.10	107.40	4	5
A	42	ASN	CB-CG-ND2	7.38	127.47	116.40	1	2
A	93	GLU	C-CA-CB	7.29	123.95	110.10	4	1
A	65	ASP	CA-CB-CG	7.29	119.89	112.60	1	5
A	154	TRP	CG-CD2-CE2	7.23	98.52	107.20	8	6
A	154	TRP	CB-CG-CD2	7.23	116.68	126.80	3	2
A	147	THR	CA-CB-CG2	7.17	122.69	110.50	5	1
A	64	GLU	CB-CG-CD	7.17	124.78	112.60	5	1
A	157	GLN	OE1-CD-NE2	7.13	115.47	122.60	7	3
A	99	ILE	CA-CB-CG2	7.08	122.54	110.50	1	2
A	115	THR	CA-CB-OG1	7.06	99.02	109.60	7	3
A	93	GLU	CB-CG-CD	7.04	124.57	112.60	2	3
A	157	GLN	CG-CD-NE2	7.02	126.94	116.40	4	1
A	16	ALA	C-CA-CB	7.02	99.97	110.50	3	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	106	ALA	N-CA-CB	6.99	99.91	110.40	4	2
A	37	SER	O-C-N	6.99	134.18	123.00	4	3
A	45	THR	CA-CB-OG1	6.93	99.21	109.60	9	4
A	121	HIS	O-C-N	6.90	111.96	123.00	8	2
A	62	ASP	C-N-CA	6.88	134.09	121.70	10	1
A	154	TRP	CB-CG-CD1	6.86	116.62	126.90	7	5
A	72	ALA	O-C-N	6.85	133.96	123.00	3	1
A	159	LYS	C-CA-CB	6.81	123.04	110.10	3	1
A	144	ASP	O-C-N	6.72	112.25	123.00	2	2
A	101	HIS	ND1-CE1-NE2	6.65	115.05	108.40	6	2
A	37	SER	CA-C-N	6.63	102.94	116.20	9	2
A	61	THR	CA-CB-OG1	6.61	99.69	109.60	4	1
A	103	TYR	O-C-N	6.60	112.43	123.00	2	1
A	95	PHE	CA-CB-CG	6.50	107.30	113.80	5	3
A	137	VAL	CA-CB-CG1	6.50	99.36	110.40	9	1
A	142	ASN	CB-CG-ND2	6.49	126.14	116.40	6	2
A	34	ALA	C-CA-CB	6.45	100.82	110.50	3	2
A	143	GLN	CG-CD-NE2	6.44	126.07	116.40	5	4
A	105	LYS	CG-CD-CE	6.42	126.06	111.30	2	2
A	150	ARG	NE-CZ-NH2	6.42	124.97	119.20	8	4
A	41	PHE	N-CA-CB	6.42	121.41	110.50	8	1
A	157	GLN	CB-CG-CD	6.37	123.44	112.60	4	1
A	44	PHE	CA-CB-CG	6.33	120.13	113.80	2	4
A	105	LYS	CA-CB-CG	6.33	101.45	114.10	3	1
A	100	PHE	CB-CG-CD2	6.29	110.01	120.70	3	1
A	9	THR	CA-CB-OG1	6.28	119.02	109.60	6	2
A	66	PHE	CA-CB-CG	6.27	120.07	113.80	8	2
A	94	THR	CA-CB-OG1	6.26	100.21	109.60	3	4
A	156	GLU	CB-CG-CD	6.24	123.21	112.60	2	1
A	74	ASP	CA-CB-CG	6.21	118.81	112.60	8	3
A	60	GLN	CA-CB-CG	6.20	126.51	114.10	8	2
A	21	ILE	CA-CB-CG1	6.20	120.95	110.40	3	2
A	74	ASP	CA-C-N	6.19	103.81	116.20	3	1
A	25	ILE	N-CA-CB	6.18	122.01	111.50	4	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	51	ALA	CA-C-N	6.18	126.17	116.90	10	2
A	20	LYS	CB-CG-CD	6.17	125.49	111.30	4	1
A	102	ILE	N-CA-CB	6.16	101.03	111.50	9	1
A	161	SER	O-C-N	6.15	113.16	123.00	8	2
A	90	THR	CA-CB-OG1	6.13	100.41	109.60	1	3
A	56	ALA	C-CA-CB	6.12	101.32	110.50	2	2

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	4.15	10
2	4.98	12
3	3.32	8
4	5.81	14
5	1.66	4
6	6.64	16
7	3.32	8
8	2.90	7
9	6.22	15
10	6.22	15

There are 109 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:150:ARG:HG3	A:151:ILE:HG13	0.94	10	1
A:33:VAL:HG21	A:67:LEU:HD21	0.79	4	1
A:75:PHE:HB2	A:106:ALA:HA	0.71	10	2
A:80:ILE:HD12	A:111:VAL:HG12	0.70	6	1
A:118:ASP:HA	A:136:LEU:HD13	0.70	2	1
A:59:LEU:HB2	A:94:THR:HG21	0.66	1	1
A:46:LYS:HD3	A:155:VAL:HG21	0.65	10	1
A:143:GLN:HB2	A:150:ARG:HG2	0.64	9	1
A:7:PHE:HA	A:50:VAL:O	0.63	9	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:83:VAL:HG12	A:136:LEU:HD12	0.61	8	1
A:3:ILE:HD13	A:81:GLY:HA3	0.61	3	1
A:6:PHE:HA	A:31:VAL:HG22	0.60	2	1
A:137:VAL:HG23	A:143:GLN:HB3	0.60	10	1
A:36:ALA:HA	A:41:PHE:HB2	0.58	9	1
A:21:ILE:O	A:25:ILE:HG12	0.58	3	2
A:5:ILE:HD11	A:26:GLY:HA3	0.57	1	1
A:95:PHE:HB2	A:122:PHE:HB3	0.57	2	1
A:81:GLY:HA2	A:112:VAL:HB	0.57	10	1
A:82:LEU:HD12	A:114:GLN:HB2	0.56	4	1
A:52:PRO:HG3	A:60:GLN:HB2	0.56	7	1
A:122:PHE:HE1	A:128:VAL:HG22	0.55	5	1
A:18:ALA:HB1	A:155:VAL:HG11	0.55	3	1
A:67:LEU:HB3	A:101:HIS:CD2	0.54	1	1
A:155:VAL:HG23	A:163:ALA:HB3	0.54	5	1
A:67:LEU:HB3	A:101:HIS:HD2	0.53	1	1
A:47:VAL:HB	A:82:LEU:HD23	0.53	6	1
A:147:THR:HA	A:154:TRP:HZ2	0.53	1	1
A:25:ILE:HG23	A:153:LYS:HA	0.53	10	1
A:82:LEU:HD12	A:114:GLN:H	0.53	4	1
A:79:THR:HA	A:110:LYS:O	0.52	4	2
A:5:ILE:HD12	A:50:VAL:HG21	0.52	10	1
A:7:PHE:HB2	A:30:VAL:HG12	0.52	7	1
A:101:HIS:O	A:104:GLU:HB3	0.52	3	1
A:137:VAL:HB	A:146:LEU:HD12	0.52	10	1
A:82:LEU:HB2	A:135:GLY:HA2	0.52	10	1
A:95:PHE:HZ	A:127:ALA:HB2	0.51	10	1
A:117:THR:HB	A:135:GLY:HA3	0.51	9	1
A:139:ASP:HA	A:154:TRP:HZ2	0.51	4	1
A:110:LYS:HE3	A:132:LYS:O	0.50	2	1
A:32:ASP:HB3	A:35:LYS:HB2	0.50	5	1
A:3:ILE:HG22	A:5:ILE:HG23	0.50	10	1
A:154:TRP:CD1	A:154:TRP:H	0.49	2	1
A:81:GLY:O	A:83:VAL:HG23	0.49	2	1
A:52:PRO:HB2	A:58:ASP:HB3	0.49	7	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:61:THR:HA	A:64:GLU:HB3	0.49	7	1
A:31:VAL:HG23	A:63:TRP:HZ3	0.48	6	1
A:63:TRP:HB2	A:67:LEU:HD12	0.48	1	1
A:71:GLU:HA	A:101:HIS:HE1	0.48	4	1
A:3:ILE:HD11	A:139:ASP:HB3	0.48	5	1
A:5:ILE:HG23	A:30:VAL:HA	0.48	4	1
A:94:THR:HA	A:123:GLU:HB3	0.48	6	1
A:5:ILE:HG13	A:22:SER:HB3	0.48	1	1
A:80:ILE:HG12	A:108:ALA:HB2	0.48	8	1
A:117:THR:HG23	A:143:GLN:HG2	0.47	6	1
A:121:HIS:CE1	A:131:GLY:HA2	0.47	4	1
A:5:ILE:HG23	A:50:VAL:HG21	0.47	9	1
A:128:VAL:O	A:130:GLY:N	0.46	3	1
A:82:LEU:HD13	A:134:VAL:HB	0.46	3	1
A:35:LYS:O	A:39:GLU:HB3	0.46	8	1
A:3:ILE:HG23	A:46:LYS:HB2	0.46	6	1
A:6:PHE:HD1	A:31:VAL:HG13	0.46	2	1
A:80:ILE:HB	A:111:VAL:HG23	0.45	1	1
A:10:ASP:HA	A:52:PRO:HG2	0.45	9	1
A:80:ILE:HD12	A:111:VAL:CG1	0.45	6	1
A:52:PRO:HB2	A:60:GLN:HB3	0.45	6	1
A:157:GLN:HB3	A:160:GLY:HA3	0.45	9	1
A:44:PHE:CE2	A:49:LEU:HD13	0.45	10	1
A:146:LEU:HD13	A:151:ILE:HD12	0.45	10	1
A:7:PHE:CZ	A:15:GLU:HG3	0.44	7	1
A:122:PHE:HB2	A:133:PHE:HB3	0.44	9	1
A:83:VAL:HG12	A:85:LEU:HG	0.44	6	1
A:129:GLU:HB2	A:132:LYS:HB2	0.43	6	1
A:100:PHE:HA	A:103:TYR:HD2	0.43	9	1
A:77:ASN:H	A:108:ALA:HB3	0.43	9	1
A:80:ILE:O	A:111:VAL:HA	0.43	9	1
A:78:LYS:HA	A:78:LYS:HD2	0.43	1	1
A:91:TYR:HB3	A:94:THR:O	0.43	4	1
A:117:THR:HB	A:133:PHE:HB2	0.43	4	1
A:8:GLY:HA2	A:60:GLN:HE22	0.42	6	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:45:THR:O	A:76:ALA:HB1	0.42	2	1
A:107:LYS:HA	A:107:LYS:HD2	0.42	10	1
A:5:ILE:CG2	A:85:LEU:HD11	0.42	3	1
A:51:ALA:HA	A:52:PRO:HD2	0.42	8	1
A:91:TYR:O	A:93:GLU:N	0.42	3	1
A:142:ASN:ND2	A:143:GLN:OE1	0.42	4	1
A:5:ILE:HD12	A:30:VAL:HG22	0.42	7	1
A:80:ILE:HG13	A:111:VAL:HG22	0.42	9	1
A:82:LEU:HB2	A:137:VAL:HG11	0.42	9	1
A:120:TYR:HB3	A:122:PHE:CZ	0.42	1	1
A:10:ASP:HA	A:58:ASP:HA	0.41	8	1
A:77:ASN:N	A:108:ALA:HB3	0.41	9	1
A:85:LEU:HA	A:85:LEU:HD23	0.41	4	1
A:96:ALA:HB1	A:101:HIS:ND1	0.41	8	1
A:118:ASP:HA	A:136:LEU:CD1	0.41	2	1
A:83:VAL:HG22	A:154:TRP:CD1	0.41	2	1
A:154:TRP:CD1	A:154:TRP:N	0.41	2	1
A:36:ALA:HA	A:40:GLN:HB2	0.41	6	1
A:150:ARG:HA	A:153:LYS:HB2	0.41	4	1
A:44:PHE:HD2	A:47:VAL:HG13	0.41	10	1
A:31:VAL:HG23	A:63:TRP:CZ3	0.41	6	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	161	113	36	12
2	161	130	25	6
3	161	120	29	12
4	161	122	32	7
5	161	121	26	14
6	161	113	40	8
7	161	132	20	9
8	161	119	36	6
9	161	125	25	11
10	161	130	20	11

There are 64 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	125	SER	5
A	89	ASP	4
A	148	ASP	4
A	38	LYS	3
A	52	PRO	3
A	92	SER	3
A	99	ILE	3
A	113	GLY	3
A	130	GLY	3
A	154	TRP	3
A	53	THR	2
A	55	GLY	2
A	59	LEU	2
A	77	ASN	2
A	140	GLU	2
A	142	ASN	2
A	150	ARG	2
A	159	LYS	2
A	2	LYS	1
A	3	ILE	1
A	9	THR	1
A	12	GLY	1
A	13	ASN	1
A	14	ALA	1
A	26	GLY	1
A	37	SER	1
A	43	SER	1
A	44	PHE	1
A	56	ALA	1
A	61	THR	1
A	62	ASP	1
A	63	TRP	1
A	65	ASP	1
A	66	PHE	1

Chain	Res	Type	Models (Total)
A	67	LEU	1
A	68	GLY	1
A	72	ALA	1
A	73	SER	1
A	83	VAL	1
A	91	TYR	1
A	96	ALA	1
A	97	GLU	1
A	100	PHE	1
A	106	ALA	1
A	108	ALA	1
A	114	GLN	1
A	116	SER	1
A	117	THR	1
A	119	GLY	1
A	123	GLU	1
A	124	ALA	1
A	129	GLU	1
A	132	LYS	1
A	134	VAL	1
A	136	LEU	1
A	137	VAL	1
A	141	ASP	1
A	143	GLN	1
A	144	ASP	1
A	146	LEU	1
A	147	THR	1
A	149	GLU	1
A	151	ILE	1
A	152	SER	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	126	107	10	9


Model ID	Analysed	Favored	Allowed	Outliers
2	126	108	13	5
3	126	101	17	8
4	126	108	12	6
5	126	104	14	8
6	126	101	15	10
7	126	99	19	8
8	126	111	7	8
9	126	102	17	7
10	126	110	13	3

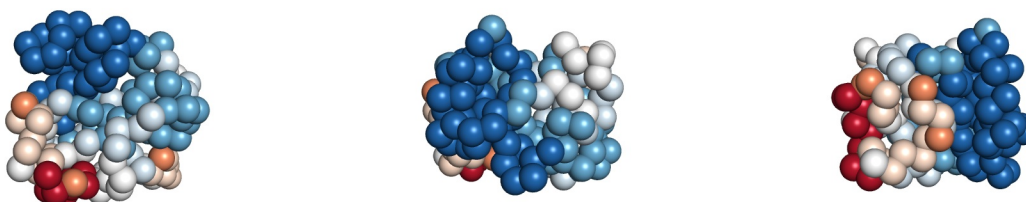
There are 51 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	147	THR	5
A	60	GLN	3
A	61	THR	3
A	69	THR	3
A	79	THR	3
A	90	THR	3
A	25	ILE	2
A	42	ASN	2
A	44	PHE	2
A	45	THR	2
A	116	SER	2
A	117	THR	2
A	137	VAL	2
A	5	ILE	1
A	7	PHE	1
A	9	THR	1
A	17	ILE	1
A	27	ASN	1
A	32	ASP	1
A	33	VAL	1
A	39	GLU	1
A	41	PHE	1
A	47	VAL	1

Chain	Res	Type	Models (Total)
A	48	ILE	1
A	49	LEU	1
A	50	VAL	1
A	52	PRO	1
A	53	THR	1
A	59	LEU	1
A	63	TRP	1
A	67	LEU	1
A	73	SER	1
A	77	ASN	1
A	78	LYS	1
A	80	ILE	1
A	82	LEU	1
A	83	VAL	1
A	85	LEU	1
A	88	GLN	1
A	92	SER	1
A	93	GLU	1
A	102	ILE	1
A	110	LYS	1
A	112	VAL	1
A	114	GLN	1
A	115	THR	1
A	134	VAL	1
A	136	LEU	1
A	138	ILE	1
A	151	ILE	1
A	156	GLU	1

PrISM precision analysis ?

Regions of **low**  **high** precision, defined as the variability among the models that satisfy the input data and calculated as the density-weighted root mean-square fluctuation (RMSF) from the bead/atom center of density, annotated and visualized using PrISM. The per-bead precision is computed from the deposited ensemble of superposed integrative models. High- and low-precision regions are then determined by clustering beads of similar precision based on their proximity in the structure. Only coarse-grained beads (or CA atoms for atomic models) of deposited models are used for assessment and visualization, and three projections for each representative model are generated. PrISM analysis for Ensemble 1 (models deposited/total: 10/10).



Fit of model to data used for modeling ?

Mutagenesis

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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