

Integrative Structure Validation Report ?

February 18, 2025 - 08:46 AM 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	9A8X
Structure Title	Complex structure of holo-GmHO-1 and Ferredoxin III from maize root
Structure Authors	Tohd, R.; Yu, J.; Kurisu, G.
Deposited on	2024-10-16

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

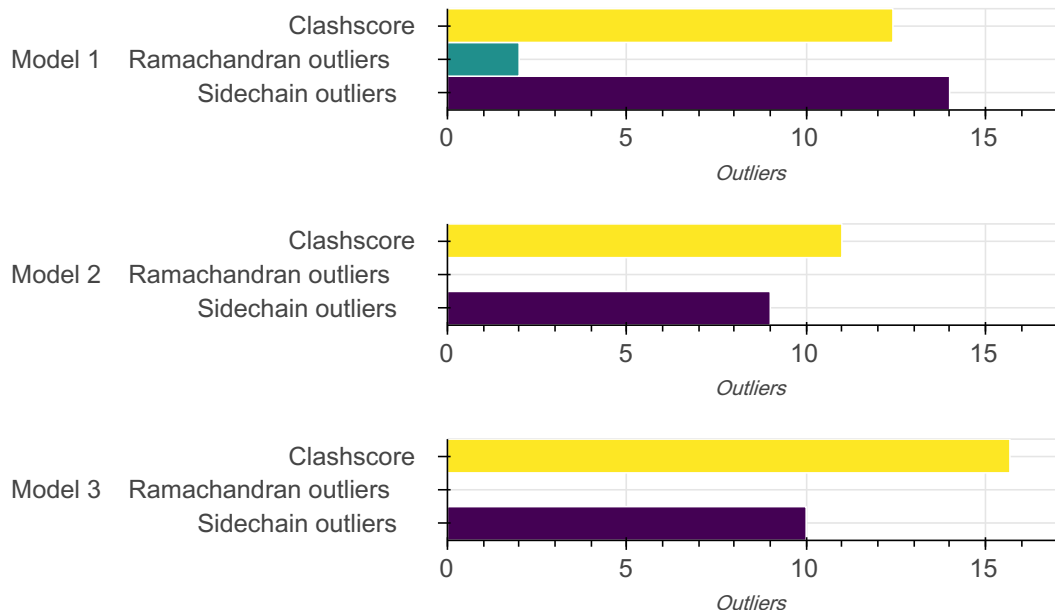
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 3 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	1-3	1	Heme oxygenase (biliverdin-producing)	A	211	-	1-211	100.00 / 100.00	Atomic
		2	Ferredoxin-3, chloroplastic	B	97	-	1-97	100.00 / 100.00	Atomic
		3	FE2/S2 (INORGANIC) CLUSTER	C	Non-polymeric	-	-	Not available / Not available	Atomic

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		4	PROTOPORPHYRIN IX CONTAINING FE	D	Non-polymeric	-	-	Not available / Not available	Atomic

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
1	NMR data	BMRB	26301
2	Experimental model	PDB	7CKA
3	Experimental model	PDB	5H57

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	docking	None	A docking simulation was performed with holo-GmHO-1 (Protein Data Bank [PDB] ID:7CKA) and maize Fd (Protein Data Bank [PDB] ID: 5h57) using the HADDOCK server based on NMR chemical shift perturbation experiments of apo-GmHO-1. Ten HADDOCK models were successfully obtained, from which the top cluster of models with a HADDOCK score of -57.0 +/- 2.2 were adopted.	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.40	model building	https://rascar.science.uu.nl/haddock2.4/

Data quality ?

NMR

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 no bond length outliers.

Standard geometry: angle outliers ?

There are 3 bond angle outliers in this entry (0.03% of 10459 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D	1	HEM	C3B-CAB-CBB	4.27	132.82	120.00	3	3

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	12.42	61
2	11.00	54
3	15.68	77

There are 192 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)
B:42:ALA:CB	D:1:HEM:O1A	1.44	2	3
A:5:GLU:CG	B:38:TYR:O	1.32	3	1
B:42:ALA:HB2	D:1:HEM:CGA	1.31	3	3
A:21:ARG:NH1	B:24:TYR:CD2	1.30	2	1
B:43:GLY:HA2	C:1:FES:S1	1.29	1	1
A:5:GLU:HG2	B:38:TYR:O	1.28	3	1
B:42:ALA:HB2	D:1:HEM:O2A	1.27	3	2
B:42:ALA:CB	D:1:HEM:CGA	1.17	3	2
A:21:ARG:NH1	B:24:TYR:HD2	1.13	2	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:42:ALA:HB1	D:1:HEM:O1A	1.11	2	2
B:42:ALA:HB2	D:1:HEM:O1A	1.09	2	2
A:170:GLN:OE1	B:45:CYS:HB2	1.07	3	2
B:43:GLY:CA	C:1:FES:S1	1.05	1	1
A:5:GLU:CD	B:38:TYR:O	1.03	3	1
A:8:ARG:NH1	B:41:ARG:HD3	1.03	2	1
A:21:ARG:HD2	B:27:ASP:OD2	0.95	2	1
B:45:CYS:SG	C:1:FES:FE2	0.94	1	1
B:45:CYS:HG	C:1:FES:FE2	0.93	1	1
A:8:ARG:CZ	B:41:ARG:HB2	0.93	2	2
A:21:ARG:NH1	B:24:TYR:CE2	0.84	2	1
B:41:ARG:HA	B:78:CYS:HB2	0.79	1	1
A:170:GLN:OE1	B:45:CYS:CB	0.79	3	1
A:166:PRO:HA	B:44:ALA:HB1	0.79	2	1
A:173:ARG:NH2	B:40:CYS:HB2	0.77	2	2
A:5:GLU:OE1	B:38:TYR:O	0.76	3	1
A:8:ARG:HH21	D:1:HEM:HAA2	0.76	3	1
A:5:GLU:HG2	B:38:TYR:C	0.75	3	1
A:4:VAL:HB	B:39:SER:OG	0.73	3	1
A:123:ALA:HB1	A:194:GLU:HG2	0.73	3	3
A:173:ARG:CZ	B:40:CYS:HB3	0.71	3	2
A:8:ARG:NH2	D:1:HEM:HAA2	0.71	3	1
A:21:ARG:HD2	A:22:GLU:HG3	0.70	1	1
A:61:LYS:HE2	A:65:GLU:OE2	0.70	1	3
A:8:ARG:HH12	B:41:ARG:HD3	0.69	2	1
A:8:ARG:HH11	B:41:ARG:HD3	0.69	3	1
A:21:ARG:NH1	B:27:ASP:OD2	0.68	3	1
A:16:THR:HG21	A:32:GLU:HB3	0.67	3	3
B:40:CYS:HA	D:1:HEM:O2D	0.67	1	3
B:42:ALA:CB	D:1:HEM:O2A	0.66	3	1
A:173:ARG:CZ	B:40:CYS:CB	0.65	3	2
B:52:ILE:HD13	B:88:ILE:HG12	0.64	3	3
A:4:VAL:HG11	A:173:ARG:HD3	0.63	3	1
B:24:TYR:CD2	B:79:VAL:HA	0.63	1	1
A:8:ARG:NE	B:40:CYS:O	0.62	2	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:42:ALA:HB1	D:1:HEM:CGA	0.62	3	1
A:5:GLU:HG2	B:39:SER:HA	0.62	3	1
B:44:ALA:N	C:1:FES:S1	0.62	1	1
A:144:LYS:O	A:148:GLU:HG3	0.60	3	3
A:21:ARG:NH2	B:27:ASP:OD2	0.60	3	1
B:45:CYS:SG	C:1:FES:S2	0.60	1	1
A:8:ARG:HD2	B:41:ARG:HB2	0.59	3	1
A:165:LEU:HB3	A:166:PRO:HD3	0.58	1	3
A:29:GLN:NE2	A:31:GLU:HB3	0.58	2	3
A:8:ARG:NE	B:41:ARG:HB2	0.57	3	1
A:8:ARG:NE	D:1:HEM:HAD1	0.57	1	2
A:91:TRP:O	A:95:GLN:HG2	0.57	1	3
B:40:CYS:O	D:1:HEM:O2D	0.57	2	2
B:24:TYR:HD2	B:79:VAL:HA	0.56	1	1
A:8:ARG:HG3	D:1:HEM:HAD2	0.56	2	2
B:37:PRO:HB2	B:47:THR:HG22	0.55	1	1
B:66:ASP:O	B:70:GLN:HG3	0.55	1	1
A:151:LEU:HB3	A:154:LYS:HB3	0.55	2	3
A:8:ARG:HG2	D:1:HEM:CAD	0.54	3	1
A:8:ARG:HG2	D:1:HEM:HAD2	0.54	3	1
A:173:ARG:NE	B:40:CYS:HB3	0.53	3	1
A:8:ARG:CD	B:41:ARG:HB2	0.53	3	1
A:21:ARG:CZ	B:27:ASP:OD2	0.52	3	1
B:41:ARG:O	B:79:VAL:HG13	0.52	1	1
B:43:GLY:C	C:1:FES:S1	0.51	1	1
A:71:TYR:OH	A:121:PRO:HA	0.50	3	3
B:39:SER:HB3	B:45:CYS:SG	0.50	1	1
A:173:ARG:NH2	B:40:CYS:HB3	0.50	1	1
B:46:SER:HB2	B:93:GLU:HG3	0.49	1	1
A:40:PRO:HB3	A:209:ILE:HG22	0.49	1	3
A:29:GLN:HE22	A:31:GLU:HB3	0.49	3	2
A:21:ARG:HH11	B:24:TYR:HD2	0.49	2	1
B:9:GLY:HA3	B:13:GLU:CD	0.49	1	1
A:8:ARG:CZ	B:41:ARG:CB	0.49	3	1
B:24:TYR:HB2	B:27:ASP:OD1	0.49	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:40:CYS:O	D:1:HEM:O2A	0.49	1	1
A:173:ARG:NH2	B:40:CYS:CB	0.49	2	1
A:152:ASN:O	A:153:ASN:HB2	0.48	3	3
A:8:ARG:HE	D:1:HEM:HAD1	0.48	1	1
A:8:ARG:NH1	B:41:ARG:CB	0.48	3	1
A:125:ILE:HD12	A:183:TRP:CZ2	0.48	3	3
A:173:ARG:HA	A:176:LEU:HD12	0.47	3	2
A:147:ALA:HA	A:151:LEU:HB2	0.47	3	3
A:173:ARG:CZ	B:40:CYS:HB2	0.47	2	2
A:125:ILE:HD12	A:183:TRP:HZ2	0.47	1	2
A:142:ILE:HD11	D:1:HEM:CBB	0.46	3	1
A:35:VAL:HA	A:38:TRP:CD1	0.46	2	3
B:59:GLN:NE2	B:76:LEU:H	0.46	2	2
A:8:ARG:NH1	A:12:MET:HG3	0.46	3	1
A:133:PHE:HB3	D:1:HEM:HBD1	0.46	3	1
A:104:SER:HB3	A:105:PRO:HD3	0.45	2	3
A:143:GLY:HA3	A:159:TYR:CZ	0.45	3	3
A:4:VAL:CB	B:39:SER:OG	0.44	3	1
A:8:ARG:NH2	B:41:ARG:HB2	0.44	2	1
A:8:ARG:NH1	B:41:ARG:HB3	0.44	3	1
A:126:CYS:HB2	A:191:CYS:SG	0.43	1	2

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	304	284	18	2
2	304	293	11	0
3	304	293	11	0

There are 2 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
B	45	CYS	1
B	46	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	265	234	17	14
2	265	243	13	9
3	265	243	12	10

There are 16 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	29	GLN	3
A	31	GLU	3
A	36	THR	3
A	43	GLU	3
A	70	SER	3
A	84	SER	3
A	136	SER	3
A	150	LEU	3
A	22	GLU	2
A	19	GLN	1
A	21	ARG	1
A	167	ARG	1
B	35	GLU	1
B	41	ARG	1
B	47	THR	1
B	79	VAL	1

Fit of model to data used for modeling ?

NMR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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