

Integrative Structure Validation Report ?

February 27, 2025 - 12:14 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

PyMOL Version 2.5.0

PDB ID	8ZZD
PDB-Dev ID	PDBDEV_00000013
Structure Title	Integrative structure of P450-Ferredoxin Complex
Structure Authors	Bowen AM; Johnson EOD; Mercuri F; Hoskins NJ; Qiao R; McCullagh JSO; Lovett JE; Bell SG; Zhou W; Timmel CR; Wong LL; Harmer JH
Deposited on	2018-01-22

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

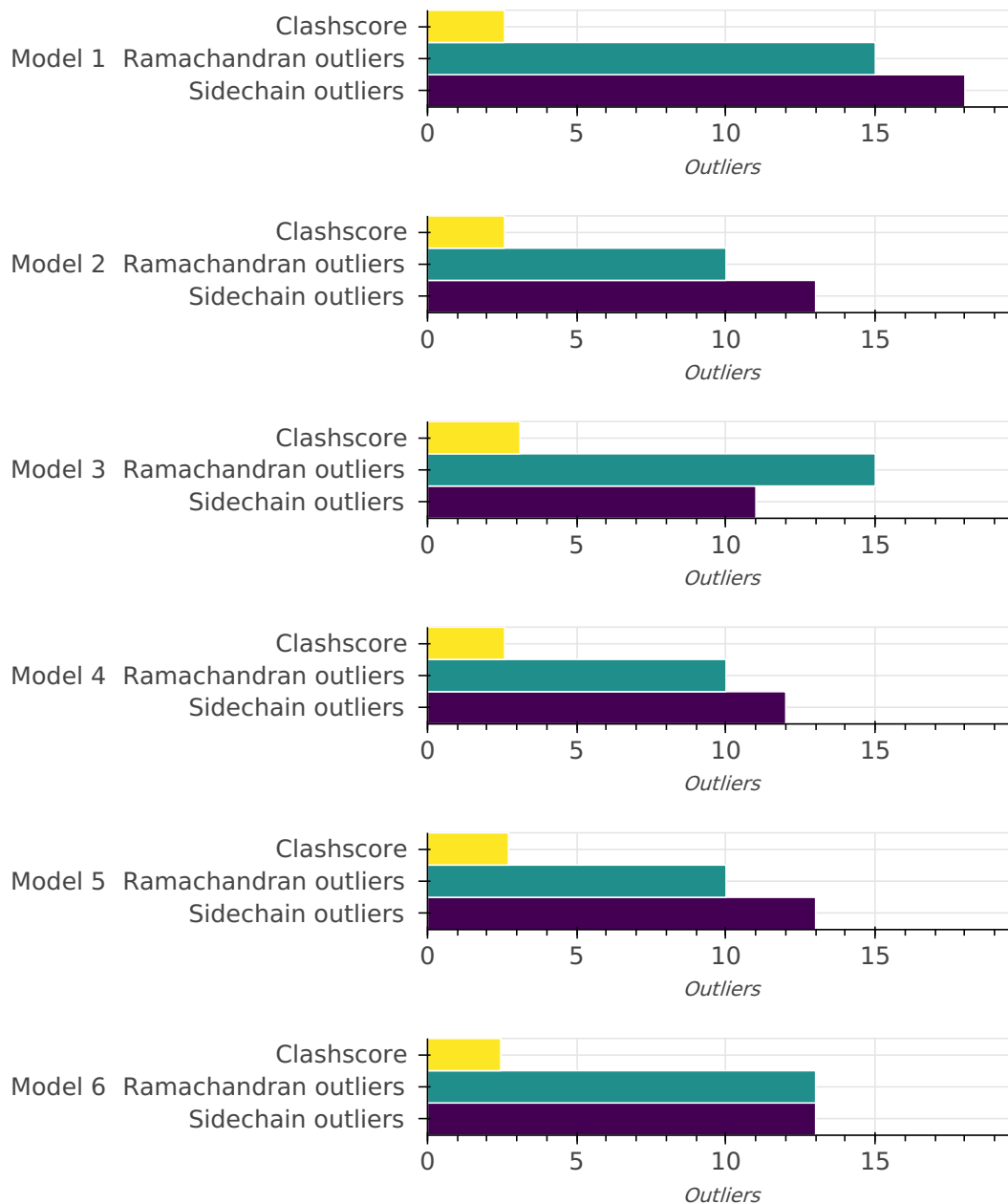
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 6 model(s). A total of 8 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	1-6	1	CYP199A2	A [A1]	399	1-399	-	100.00 / 100.00	Atomic
		2	HaPux	B [C1]	106	1-106	-	100.00 / 100.00	Atomic
		3	PROTOPORPHYRIN IX CONTAINING FE	C [A1]	Non-polymeric	-	-	Not available / Not available	Atomic
		4	4-METHOXYBENZOIC ACID	D [A1]	Non-polymeric	-	-	Not available / Not available	Atomic
		5	CHLORIDE ION	E [A1]	Non-polymeric	-	-	Not available / Not available	Atomic
		6	FE2/S2 (INORGANIC) CLUSTER	F [C1]	Non-polymeric	-	-	Not available / Not available	Atomic

Datasets used for modeling ?

There are 8 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	4DNJ
2	Experimental model	PDB	4LTU
3	EPR data	Not available	10.5287/bodleian:5zqPg5yVe
4	EPR data	Not available	10.5287/bodleian:5zqPg5yVe
5	EPR data	Not available	10.5287/bodleian:5zqPg5yVe
6	EPR data	Not available	10.5287/bodleian:5zqPg5yVe
7	EPR data	Not available	10.5287/bodleian:5zqPg5yVe
8	EPR data	Not available	10.5287/bodleian:5zqPg5yVe

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	Integrative Modeling	None	None	None	False	False

There are 5 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	PatchDock	Beta1.3	model building	https://bioinfo3d.cs.tau.ac.il/PatchDock/
2	FireDock	develop-5abded4c39	model building	http://bioinfo3d.cs.tau.ac.il/FireDock/
3	MMM	2017.10	model building	http://www.epr.ethz.ch/software.html
4	Matlab	R2017a	data processing	https://uk.mathworks.com/products/matlab.html
5	Gromacs	Not available	refinement	http://www.gromacs.org/

Data quality ?

EPR

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 109 bond length outliers in this entry (0.45% of 24030 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D	1	ANN	C5-O3	4.53	1.44	1.35	5	6
A	3	HIS	CD2-NE2	4.49	1.32	1.37	4	6
A	94	HIS	CD2-NE2	4.48	1.32	1.37	1	6
B	7	HIS	CG-ND1	4.47	1.33	1.38	2	6
A	338	HIS	CD2-NE2	4.40	1.33	1.37	1	6

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	9	HIS	CG-ND1	4.37	1.33	1.38	6	5
B	49	HIS	CD2-NE2	4.37	1.33	1.37	3	6
A	192	HIS	CD2-NE2	4.35	1.33	1.37	6	6
A	346	HIS	CG-ND1	4.35	1.33	1.38	1	6
B	7	HIS	CD2-NE2	4.33	1.33	1.37	1	6
A	338	HIS	CG-ND1	4.31	1.33	1.38	2	6
A	9	HIS	CD2-NE2	4.31	1.33	1.37	3	5
B	30	HIS	CG-ND1	4.27	1.33	1.38	6	3
A	94	HIS	CG-ND1	4.27	1.33	1.38	3	5
A	3	HIS	CG-ND1	4.26	1.33	1.38	3	4
B	49	HIS	CG-ND1	4.25	1.33	1.38	1	6
A	215	HIS	CG-ND1	4.23	1.33	1.38	4	6
A	346	HIS	CD2-NE2	4.19	1.33	1.37	4	6
B	30	HIS	CD2-NE2	4.18	1.33	1.37	4	4
A	192	HIS	CG-ND1	4.18	1.33	1.38	2	1
A	215	HIS	CD2-NE2	4.14	1.33	1.37	1	4

Standard geometry: angle outliers ?

There are 157 bond angle outliers in this entry (0.48% of 32784 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	21	ASP	CA-CB-CG	8.21	120.81	112.60	1	6
F	1	FES	FE1-S2-FE2	6.42	68.34	75.66	2	6
B	49	HIS	CB-CG-CD2	6.32	122.98	131.20	6	6
A	192	HIS	CB-CG-CD2	6.31	122.99	131.20	6	6
F	1	FES	S1-FE2-S2	6.18	111.38	104.33	2	6
F	1	FES	FE1-S1-FE2	6.05	68.40	75.66	2	6
A	383	ASN	CA-CB-CG	5.74	118.34	112.60	1	6
A	22	ASP	CA-CB-CG	5.73	106.87	112.60	2	4
B	49	HIS	CA-CB-CG	5.61	119.41	113.80	5	5
A	90	ASP	CA-CB-CG	5.50	118.10	112.60	1	4
B	33	ASP	C-N-CA	5.49	131.57	121.70	4	4
B	33	ASP	CA-CB-CG	5.43	118.03	112.60	1	4
A	9	HIS	CB-CG-CD2	5.40	124.18	131.20	3	6
F	1	FES	S1-FE1-S2	5.37	110.78	104.33	3	6

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	74	PHE	CA-CB-CG	5.26	119.06	113.80	5	6
B	64	ASP	CA-CB-CG	5.20	117.80	112.60	2	3
B	30	HIS	CB-CG-CD2	5.18	124.47	131.20	2	6
A	105	LEU	C-N-CA	5.06	130.81	121.70	5	4
A	222	GLU	N-CA-CB	5.04	101.93	110.50	6	1
A	346	HIS	CB-CG-CD2	4.80	124.96	131.20	5	6
A	106	SER	N-CA-C	4.76	124.34	111.00	5	5
B	66	ASN	OD1-CG-ND2	4.75	117.85	122.60	1	1
B	76	SER	C-N-CA	4.70	130.15	121.70	5	3
A	351	GLN	OE1-CD-NE2	4.62	117.98	122.60	2	2
B	48	CYS	N-CA-CB	4.56	102.76	110.50	5	6
A	319	ASP	CA-CB-CG	4.48	117.08	112.60	2	1
A	395	GLN	OE1-CD-NE2	4.48	118.12	122.60	3	1
A	210	PHE	CA-CB-CG	4.48	118.28	113.80	1	4
A	330	ASP	CA-CB-CG	4.47	117.07	112.60	2	2
A	3	HIS	CB-CG-CD2	4.41	125.46	131.20	4	4
B	7	HIS	CB-CG-CD2	4.37	125.52	131.20	4	4
A	327	ASP	CA-CB-CG	4.33	116.93	112.60	5	1
A	277	GLU	CB-CG-CD	4.26	119.85	112.60	2	2
B	77	ASP	CA-CB-CG	4.26	116.86	112.60	2	1
A	324	ASP	CA-CB-CG	4.22	116.82	112.60	2	1
A	179	ASN	CA-CB-CG	4.20	116.80	112.60	1	3
B	49	HIS	CB-CG-ND1	4.18	128.97	122.70	3	3
B	16	ASP	CA-CB-CG	4.17	116.77	112.60	2	1
A	347	MET	C-N-CA	4.14	129.16	121.70	4	1
A	2	GLN	C-N-CA	4.11	129.10	121.70	3	2
B	45	CYS	C-N-CA	4.10	129.09	121.70	4	1
B	72	ASP	CA-CB-CG	4.08	116.68	112.60	6	1
A	109	THR	CA-CB-CG2	4.07	117.41	110.50	5	1
A	192	HIS	CA-CB-CG	4.06	117.86	113.80	6	1
B	42	ASN	OD1-CG-ND2	4.04	118.56	122.60	3	1
A	180	GLU	CB-CG-CD	4.04	119.46	112.60	4	1
A	94	HIS	CB-CG-CD2	4.03	125.97	131.20	5	1
A	43	ASN	CA-CB-CG	4.00	108.60	112.60	4	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	2.58	20
2	2.58	20
3	3.10	24
4	2.58	20
5	2.71	21
6	2.45	19

There are 124 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)
A:67:ARG:HH22	A:306:GLY:HA2	0.71	2	6
A:347:MET:HG3	A:351:GLN:HE22	0.70	6	1
B:41:GLY:HA2	B:86:CYS:HB2	0.68	4	5
A:95:THR:HG23	B:44:VAL:HG12	0.65	3	2
B:24:MET:HE3	B:28:LEU:HD12	0.64	1	2
A:168:ALA:HB1	A:241:ASP:HB2	0.62	6	5
A:87:LEU:HD13	C:1:HEM:HAD2	0.60	6	6
B:75:ALA:HB1	B:104:ARG:HG2	0.56	6	1
A:63:PHE:HB3	A:290:ARG:HB3	0.53	1	6
A:290:ARG:HH21	A:346:HIS:CD2	0.53	6	3
B:46:ALA:HB1	B:74:THR:HA	0.52	1	1
A:71:LEU:HD13	A:177:PRO:HB3	0.50	5	4
B:94:LEU:HD22	B:97:LEU:HD13	0.50	4	6
A:173:ASN:HA	A:384:ASN:HB2	0.50	1	6
A:128:LEU:HD11	A:141:LEU:HD13	0.49	6	6
A:174:ALA:HA	A:182:ARG:HG3	0.49	6	5
A:36:VAL:HG11	A:303:ILE:HD11	0.49	4	2
A:380:ARG:HG3	A:388:GLY:O	0.49	5	4
A:110:MET:HG3	A:352:LEU:HB3	0.49	4	1
A:36:VAL:HG22	A:47:VAL:HG12	0.48	4	3
A:350:GLY:HA3	C:1:HEM:C3C	0.47	6	5
A:171:VAL:HG11	D:1:ANN:H3	0.47	6	4

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:381:ARG:HE	A:390:GLU:HG3	0.46	6	1
A:49:ARG:HB2	A:52:GLU:OE1	0.46	3	1
A:350:GLY:HA3	C:1:HEM:C4C	0.46	3	3
A:67:ARG:HA	A:74:PHE:HB2	0.46	4	3
A:30:LEU:HD22	A:37:VAL:HG21	0.45	1	2
A:73:ASP:HB3	A:76:LYS:HD2	0.44	3	2
A:85:LEU:HB3	A:97:THR:HG21	0.44	5	2
A:344:GLY:HA2	B:42:ASN:ND2	0.44	3	1
B:71:LEU:HD22	B:82:SER:HB3	0.43	2	2
B:104:ARG:HD3	B:106:THR:O	0.43	1	1
A:81:ARG:HH22	D:1:ANN:C1	0.43	3	2
A:62:THR:HG21	A:296:VAL:HG11	0.43	1	1
A:167:TYR:HB2	A:192:HIS:HB3	0.42	2	1
A:319:ASP:HA	A:320:PRO:HD2	0.42	2	3
A:290:ARG:HA	A:290:ARG:HD3	0.42	1	3
B:21:ASP:O	B:90:ILE:HG13	0.41	5	1
A:80:TRP:CG	A:81:ARG:H	0.41	5	1
A:86:ILE:HG23	A:87:LEU:H	0.41	3	1
A:82:PRO:HA	A:83:PRO:HD3	0.41	3	1
A:138:ILE:HA	A:142:ALA:HB3	0.41	5	2
A:200:CYS:SG	A:233:ARG:HB2	0.41	5	1
B:37:ALA:HB1	B:40:GLY:HA2	0.41	2	1
A:13:ASP:HA	A:14:PRO:HD2	0.41	3	1
A:341:PHE:HB3	A:348:CYS:HB3	0.40	3	1
A:12:ILE:HG23	A:26:GLU:OE2	0.40	4	1
A:98:ARG:HD3	C:1:HEM:O2D	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	501	440	46	15
2	501	453	38	10
3	501	448	38	15
4	501	448	43	10
5	501	455	36	10

Model ID	Analysed	Favored	Allowed	Outliers
6	501	454	34	13

There are 24 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	336	SER	6
A	348	CYS	6
B	33	ASP	6
A	3	HIS	5
A	106	SER	5
A	134	ASN	5
A	284	PRO	5
A	35	PRO	4
A	69	VAL	4
B	77	ASP	4
A	43	ASN	3
A	239	GLY	3
A	281	PHE	3
A	115	ASP	2
B	19	ILE	2
B	46	ALA	2
A	5	ALA	1
A	21	ALA	1
A	94	HIS	1
A	95	THR	1
A	116	GLY	1
B	18	ALA	1
B	37	ALA	1
B	43	ALA	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	401	360	23	18
2	401	362	26	13
3	401	357	33	11

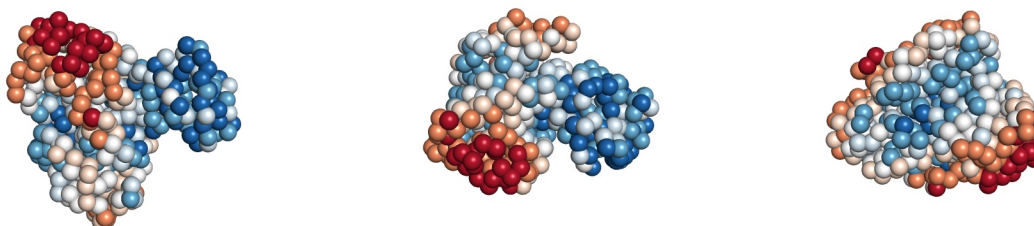
Model ID	Analysed	Favored	Allowed	Outliers
4	401	365	24	12
5	401	360	28	13
6	401	362	26	13

There are 28 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	192	HIS	6
A	287	THR	6
A	291	THR	6
A	122	ASP	5
A	237	SER	5
A	22	ASP	4
B	21	ASP	4
B	49	HIS	4
A	2	GLN	3
A	71	LEU	3
A	95	THR	3
A	109	THR	3
A	127	GLU	3
B	1	PRO	3
B	104	ARG	3
A	134	ASN	2
A	199	GLN	2
A	224	THR	2
A	225	PRO	2
A	302	THR	2
B	95	ASP	2
A	226	GLU	1
A	297	GLU	1
A	332	THR	1
B	16	ASP	1
B	24	MET	1
B	72	ASP	1
B	106	THR	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: 6/6).



Fit of model to data used for modeling ?

EPR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.