

Integrative Structure Validation Report ?

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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	9A00
PDB-Dev ID	PDBDEV_00000036
Structure Title	Structure of the human myeloid-derived growth factor (hMYDGF) engaging the chicken KDEL receptor 2 (cKDEL2)
Structure Authors	Bortnov V; Tonelli M; Lee W; Lin Z; Annis DS; Demerdash ON; Bateman A; Mitchell JC; Ge Y; Markley JL; Mosher DF
Deposited on	2019-10-21

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

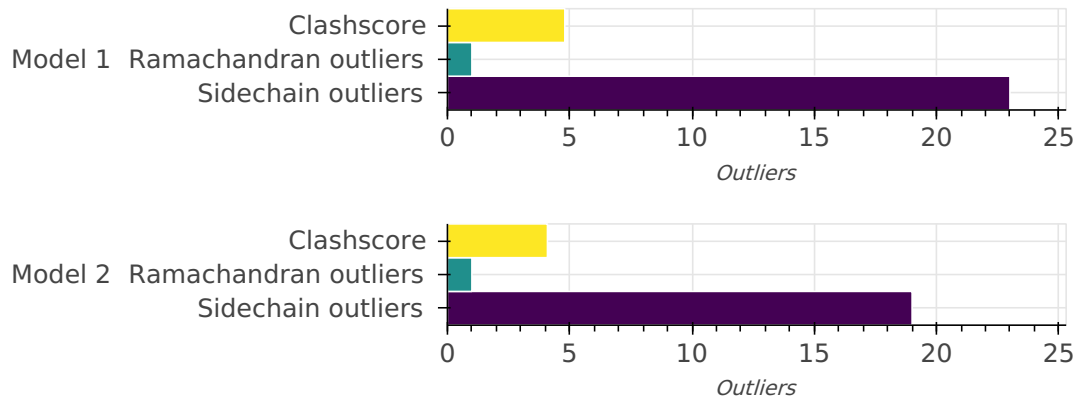
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 2 model(s). A total of 2 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	1-2	1	ER lumen protein-retaining receptor 2	A	207	1-207	-	100.00 / 100.00	Atomic
		2	Myeloid-derived growth factor	B	142	1-142	-	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	6O6W
2	Experimental model	PDB	6I6H

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	–	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	Not available	molecular docking	http://haddock.science.uu.nl/services/HADDOCK/

Data quality ?

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 no bond angle outliers.

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	4.80	27
2	4.09	23

There are 50 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:22:LYS:HG3	A:147:ILE:HG21	0.78	2	1
A:100:VAL:HB	A:101:PRO:HD3	0.72	1	2
B:60:THR:HG22	B:134:VAL:HG12	0.69	2	1
A:163:LEU:HD23	A:166:TRP:HZ3	0.64	1	1
B:48:MET:HG2	B:63:ILE:HG12	0.63	1	1
B:106:LYS:HB3	B:109:GLU:HG3	0.61	1	1
A:120:TRP:HZ2	B:140:THR:HA	0.59	2	1
B:96:ALA:HB2	B:102:ASP:HB3	0.57	2	1
A:149:THR:HG22	A:194:PHE:HE1	0.57	1	1
B:87:GLU:HB2	B:134:VAL:HG23	0.56	2	1
B:62:THR:HG23	B:132:VAL:HB	0.55	1	2
B:24:VAL:HG12	B:26:PRO:HD2	0.55	1	2
B:60:THR:HG23	B:134:VAL:HG22	0.53	1	1
A:43:VAL:HG13	A:123:SER:HB2	0.52	1	2
A:120:TRP:CZ2	B:140:THR:HA	0.52	2	1
A:165:ASN:HD22	B:142:LEU:HD21	0.51	1	1
B:111:GLU:HB3	B:118:ALA:HB3	0.51	1	1
B:17:VAL:HG12	B:35:THR:HG22	0.51	2	1
A:47:ARG:HH12	B:142:LEU:HD13	0.49	2	1
A:185:VAL:O	A:189:VAL:HG23	0.49	2	1
A:120:TRP:O	A:124:ILE:HG12	0.49	1	1
B:113:THR:HB	B:116:ALA:O	0.48	1	1
A:127:GLU:OE2	B:142:LEU:HD11	0.48	2	1
A:165:ASN:O	A:169:ARG:HG3	0.48	2	1
A:162:TYR:CD2	B:142:LEU:HD23	0.47	1	1
A:159:ARG:HA	A:159:ARG:HD2	0.47	1	1
B:55:ASP:HB3	B:57:GLN:HG2	0.47	2	1
A:120:TRP:HZ2	B:140:THR:HB	0.46	1	1
B:113:THR:HG22	B:114:LYS:HD3	0.45	2	1
A:102:VAL:HG13	A:125:TYR:HB2	0.45	2	1
A:12:HIS:HB2	A:158:TYR:CD1	0.44	1	1
B:59:PHE:HE2	B:137:ALA:HB2	0.44	2	1
A:149:THR:HG22	A:194:PHE:CE1	0.43	1	1
A:181:VAL:O	A:185:VAL:HG23	0.43	1	1
A:123:SER:O	A:127:GLU:HB2	0.43	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:163:LEU:HA	A:166:TRP:CE3	0.43	1	1
B:78:LYS:HE2	B:119:HIS:HB3	0.43	1	1
A:106:SER:HB3	A:122:PHE:HA	0.42	1	1
B:9:PHE:O	B:45:GLN:HA	0.42	1	1
A:13:LEU:O	A:17:ILE:HG12	0.41	1	1
A:98:LEU:HD21	A:132:LEU:HD12	0.41	2	1
B:17:VAL:HG13	B:37:ALA:HB2	0.41	2	1
B:19:SER:HA	B:34:PHE:O	0.41	2	1
B:39:GLN:HB3	B:73:TYR:HD2	0.41	1	1
B:63:ILE:HD11	B:131:LEU:HD12	0.41	2	1
B:9:PHE:CE1	B:46:TRP:HB2	0.41	1	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	345	324	20	1
2	345	324	20	1

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

Chain	Res	Type	Models (Total)
A	56	ILE	1
B	2	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	302	255	24	23
2	302	260	23	19

There are 33 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	9	ASP	2
A	85	THR	2
A	92	THR	2
A	116	LEU	2

Chain	Res	Type	Models (Total)
A	128	SER	2
A	146	THR	2
A	149	THR	2
A	162	TYR	2
B	52	THR	2
A	29	CYS	1
A	53	THR	1
A	54	SER	1
A	106	SER	1
A	114	SER	1
A	117	GLU	1
A	141	THR	1
A	148	THR	1
A	159	ARG	1
A	188	THR	1
B	5	THR	1
B	17	VAL	1
B	19	SER	1
B	21	SER	1
B	29	LYS	1
B	35	THR	1
B	38	SER	1
B	42	THR	1
B	74	PHE	1
B	87	GLU	1
B	93	SER	1
B	97	PHE	1
B	140	THR	1
B	141	GLU	1

Fit of model to data used for modeling ?

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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