Full wwPDB Integrative Structure Validation Report

July 06, 2020 -- 10:10 PM

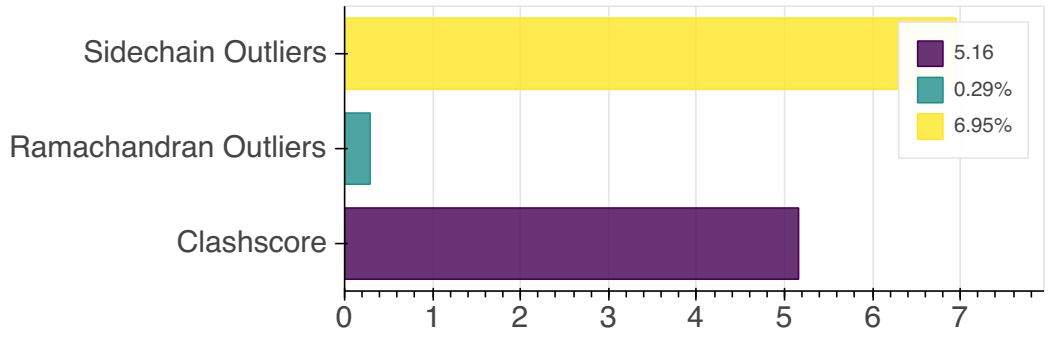
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000036
Molecule Name	Structure of the human myeloid-derived growth factor (hMYDGF) engaging the chicken KDEL receptor 2 (cKDELR2)
Title	Solution structure of human myeloid-derived growth factor suggests a conserved function in the endoplasmic reticulum
Authors	Bortnov V;Tonelli M;Lee W;Lin Z;Annis DS;Demerdash ON;Bateman A;Mitchell JC;Ge Y;Markley JL;Mosher DF

Overall quality

Model Quality: Molprobity Analysis



Ensemble information

This entry consists of 0 distinct ensemble.

Summary

This entry consists of 2 unique models, with 2 subunits in each model. A total of 2 datasets or restraints was used to build this entry. Each model is represented by 2 rigid bodies and 0 flexible or non-rigid units.

Entry composition

There are 2 unique types of models in this entry.These models are titled Cluster 1/Cluster 1 representative, Cluster 2/Cluster 2 representative respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	ER lumen protein-retaining receptor 2	A	207
1	2	2	Myeloid-derived growth factor	B	142
2	1	1	ER lumen protein-retaining receptor 2	A	207
2	2	2	Myeloid-derived growth factor	B	142

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	?	?	?	False	False

Data quality

Model quality

Standard geometry

There are 1166 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ2	1.037	0.89	39
NZ--HZ1	1.036	0.89	39
NZ--HZ3	1.037	0.89	39
NH2--HH21	0.997	0.86	23
NH1--HH12	0.999	0.86	23
NH1--HH11	0.999	0.86	23
NH2--HH22	1.002	0.86	23
OG--HG	0.961	0.84	49
OH--HH	0.96	0.84	43
OG1--HG1	0.963	0.84	55
NE--HE	0.979	0.86	23
ND2--HD21	0.979	0.86	13
NE2--HE2	0.982	0.86	13
N--H	0.976	0.86	675
SG--HG	1.325	1.2	5
NE1--HE1	0.981	0.86	11
ND1--HD1	0.983	0.86	3
ND2--HD22	0.978	0.86	13

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE21	0.977	0.86	17
NE2--HE22	0.98	0.86	17

There are 0 angle outliers in this entry.

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 the models in this entry.

Model ID	Clash score	Number of clashes
Model 1	5.16	29
Model 2	4.09	23

All 52 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Analyzed	Favored	Allowed	Outliers
1	345	324	20	1
2	345	324	20	1

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:56	ILE
2	B:33	SER

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers

Model ID	Analyzed	Favored	Allowed	Outliers
1	302	255	24	23
2	302	260	23	19

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:9	ASP
1	A:29	CYS
1	A:53	THR
1	A:54	SER
1	A:85	THR
1	A:92	THR
1	A:106	SER
1	A:114	SER
1	A:116	LEU
1	A:117	GLU
1	A:128	SER
1	A:146	THR
1	A:149	THR
1	A:162	TYR
1	B:50	SER
1	B:60	LYS
1	B:66	THR
1	B:83	THR
1	B:105	PHE

Model ID	Chain and res ID	Residue type
1	B:118	GLU
1	B:128	PHE
1	B:171	THR
1	B:172	GLU
2	A:9	ASP
2	A:85	THR
2	A:92	THR
2	A:116	LEU
2	A:128	SER
2	A:141	THR
2	A:146	THR
2	A:148	THR
2	A:149	THR
2	A:159	ARG
2	A:162	TYR
2	A:188	THR
2	B:36	THR
2	B:48	VAL
2	B:52	SER
2	B:69	SER
2	B:73	THR
2	B:83	THR
2	B:124	SER

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model