



wwPDB EM Model Validation Summary Report ⓘ

Mar 23, 2020 – 01:08 PM EDT

PDB ID : 6Q0X
EMDB ID : EMD-20555
Title : The cryo-EM structure of the SNX-BAR Mvp1 tetramer
Authors : Sun, D.; Ford, M.G.J.; Zhang, P.
Deposited on : 2019-08-02
Resolution : 4.20 Å(reported)
Based on initial models : 6H7W, 3DYT

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

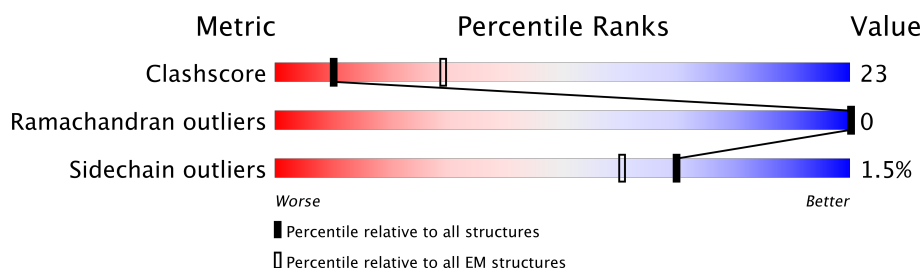
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	531	
1	B	531	
1	C	531	
1	D	531	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12468 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sorting nexin MVP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	373	Total	C	N	O	S	0	0
			3117	1996	543	566	12		
1	B	373	Total	C	N	O	S	0	0
			3117	1996	543	566	12		
1	C	373	Total	C	N	O	S	0	0
			3117	1996	543	566	12		
1	D	373	Total	C	N	O	S	0	0
			3117	1996	543	566	12		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P40959
A	-18	GLY	-	expression tag	UNP P40959
A	-17	SER	-	expression tag	UNP P40959
A	-16	SER	-	expression tag	UNP P40959
A	-15	HIS	-	expression tag	UNP P40959
A	-14	HIS	-	expression tag	UNP P40959
A	-13	HIS	-	expression tag	UNP P40959
A	-12	HIS	-	expression tag	UNP P40959
A	-11	HIS	-	expression tag	UNP P40959
A	-10	HIS	-	expression tag	UNP P40959
A	-9	SER	-	expression tag	UNP P40959
A	-8	SER	-	expression tag	UNP P40959
A	-7	GLY	-	expression tag	UNP P40959
A	-6	LEU	-	expression tag	UNP P40959
A	-5	VAL	-	expression tag	UNP P40959
A	-4	PRO	-	expression tag	UNP P40959
A	-3	ARG	-	expression tag	UNP P40959
A	-2	GLY	-	expression tag	UNP P40959
A	-1	SER	-	expression tag	UNP P40959
A	0	HIS	-	expression tag	UNP P40959
B	-19	MET	-	initiating methionine	UNP P40959
B	-18	GLY	-	expression tag	UNP P40959

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P40959
B	-16	SER	-	expression tag	UNP P40959
B	-15	HIS	-	expression tag	UNP P40959
B	-14	HIS	-	expression tag	UNP P40959
B	-13	HIS	-	expression tag	UNP P40959
B	-12	HIS	-	expression tag	UNP P40959
B	-11	HIS	-	expression tag	UNP P40959
B	-10	HIS	-	expression tag	UNP P40959
B	-9	SER	-	expression tag	UNP P40959
B	-8	SER	-	expression tag	UNP P40959
B	-7	GLY	-	expression tag	UNP P40959
B	-6	LEU	-	expression tag	UNP P40959
B	-5	VAL	-	expression tag	UNP P40959
B	-4	PRO	-	expression tag	UNP P40959
B	-3	ARG	-	expression tag	UNP P40959
B	-2	GLY	-	expression tag	UNP P40959
B	-1	SER	-	expression tag	UNP P40959
B	0	HIS	-	expression tag	UNP P40959
C	-19	MET	-	initiating methionine	UNP P40959
C	-18	GLY	-	expression tag	UNP P40959
C	-17	SER	-	expression tag	UNP P40959
C	-16	SER	-	expression tag	UNP P40959
C	-15	HIS	-	expression tag	UNP P40959
C	-14	HIS	-	expression tag	UNP P40959
C	-13	HIS	-	expression tag	UNP P40959
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C	-5	VAL	-	expression tag	UNP P40959
C	-4	PRO	-	expression tag	UNP P40959
C	-3	ARG	-	expression tag	UNP P40959
C	-2	GLY	-	expression tag	UNP P40959
C	-1	SER	-	expression tag	UNP P40959
C	0	HIS	-	expression tag	UNP P40959
D	-19	MET	-	initiating methionine	UNP P40959
D	-18	GLY	-	expression tag	UNP P40959
D	-17	SER	-	expression tag	UNP P40959
D	-16	SER	-	expression tag	UNP P40959

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP P40959
D	-14	HIS	-	expression tag	UNP P40959
D	-13	HIS	-	expression tag	UNP P40959
D	-12	HIS	-	expression tag	UNP P40959
D	-11	HIS	-	expression tag	UNP P40959
D	-10	HIS	-	expression tag	UNP P40959
D	-9	SER	-	expression tag	UNP P40959
D	-8	SER	-	expression tag	UNP P40959
D	-7	GLY	-	expression tag	UNP P40959
D	-6	LEU	-	expression tag	UNP P40959
D	-5	VAL	-	expression tag	UNP P40959
D	-4	PRO	-	expression tag	UNP P40959
D	-3	ARG	-	expression tag	UNP P40959
D	-2	GLY	-	expression tag	UNP P40959
D	-1	SER	-	expression tag	UNP P40959
D	0	HIS	-	expression tag	UNP P40959





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	49000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/3179	0.51	0/4284
1	B	0.38	0/3179	0.51	0/4284
1	C	0.38	0/3179	0.51	0/4284
1	D	0.38	0/3179	0.51	0/4284
All	All	0.38	0/12716	0.51	0/17136

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	SER	Peptide
1	B	160	SER	Peptide
1	C	160	SER	Peptide
1	D	160	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3117	0	3185	155	0
1	B	3117	0	3185	157	0
1	C	3117	0	3185	157	0
1	D	3117	0	3185	162	0
All	All	12468	0	12740	582	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 582 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:TRP:HB3	1:D:464:PHE:HZ	1.43	0.83
1:B:282:TRP:HB3	1:B:464:PHE:HZ	1.43	0.83
1:C:282:TRP:HB3	1:C:464:PHE:HZ	1.43	0.83
1:A:282:TRP:HB3	1:A:464:PHE:HZ	1.43	0.83
1:B:191:MET:HA	1:B:392:LEU:HD11	1.63	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/531 (70%)	341 (92%)	30 (8%)	0	100	100
1	B	371/531 (70%)	341 (92%)	30 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	371/531 (70%)	341 (92%)	30 (8%)	0	100	100
1	D	371/531 (70%)	341 (92%)	30 (8%)	0	100	100
All	All	1484/2124 (70%)	1364 (92%)	120 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/493 (71%)	345 (99%)	5 (1%)	69	85
1	B	350/493 (71%)	345 (99%)	5 (1%)	69	85
1	C	350/493 (71%)	344 (98%)	6 (2%)	63	83
1	D	350/493 (71%)	345 (99%)	5 (1%)	69	85
All	All	1400/1972 (71%)	1379 (98%)	21 (2%)	70	84

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	471	GLN
1	C	154	HIS
1	D	154	HIS
1	B	451	ASN
1	D	449	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.