

## wwPDB EM Validation Summary Report (i)

#### Nov 20, 2022 – 09:07 AM EST

PDB ID	:	7MBR
EMDB ID	:	EMD-23744
Title	:	Cryo-EM structure of zebrafish TRPM5 in the presence of 6 uM calcium (apo
		state)
Authors	:	Ruan, Z.; Lu, W.; Du, J.; Haley, E.
Deposited on	:	2021-04-01
Resolution	:	Not provided

This is a wwPDB EM Validation Summary Report for a publicly released PDB 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is unknown.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 of 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 <=5%

Mol	Chain	Length	Quality of chain				
1	А	1165	71%	15%	15%		
1	В	1165	71%	15%	15%		
1	С	1165	71%	15%	15%		
1	D	1165	71%	14%	15%		



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30708 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.

Mol	Chain	Residues		А	toms			AltConf	Trace	
1	Λ	006	Total	С	Ν	Ο	S	0	0	
	Л	990	7574	4963	1296	1271	44	0	0	
1	Р	006	Total	С	Ν	Ο	S	0	0	
	В	D	990	7574	4963	1296	1271	44	0	0
1	C	006	Total	С	Ν	Ο	S	0	0	
	U	990	7574	4963	1296	1271	44	0	0	
1	Л	006	Total	С	Ν	Ο	S	0	0	
	D	990	7574	4963	1296	1271	44	0	0	

• Molecule 1 is a protein called Transient receptor potential melastatin 5.

• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
2	А	1	Total         C         N         O           14         8         1         5	0
2	В	1	Total         C         N         O           14         8         1         5	0



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Mol	Chain	Residues	Atoms			AltConf	
0	С	1	Total	С	Ν	Ο	0
		1	14	8	1	5	0
0	р	1	Total	С	Ν	0	0
2	D		14	8	1	5	0

• Molecule 3 is (25R)-14beta,17beta-spirost-5-en-3beta-ol (three-letter code: YUV) (formula:  $C_{27}H_{42}O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 30 & 27 & 3 \end{array}$	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 30 & 27 & 3 \end{array}$	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 30 & 27 & 3 \end{array}$	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 30 & 27 & 3 \end{array}$	0

• Molecule 4 is (2R)-2-(hydroxymethyl)-4-{[(25R)-10alpha,14beta,17beta-spirost-5-en-3beta-y l]oxy}butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: YUY) (formula:  $C_{44}H_{72}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	AltConf
4	Λ	1	Total C O	0
4	Л	1	59  44  15	0
4	В	1	Total C O	0
4	D	1	59  44  15	0
4	С	1	Total C O	0
4	U	1	59  44  15	0
4	Л	1	Total C O	0
4	D	1	59  44  15	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Transient receptor potential melastatin 5

ASP LYS LYS LYS LYS LEU PRO PRO PHE ILE ASP ASP

• Molecule 1: Transient receptor potential melastatin 5







#### LEU PRO PHE ILE ASP HIS

• Molecule 1: Transient receptor potential melastatin 5

Chain C:	71%	15% 15%
MET VAL VAL CUSU CUSE SER SER SER SER ARG PIE CUS CUS CUS CUS CUS CUS CUS CUS CUS CUS	R44 147 147 147 147 147 163 163 163 163 165 172 173 173	L80 L94 L94 L96 L96 L96 L96 L96 L100 L100 L108 L108 L108 L108 L108 L108
9201 8210 8210 1216 1218 1218 1218 1218 1218 12218 12218 12218 12218 12218 1222 1222	1234 1241 1245 1245 1245 0248 0248 0251 1243 1248 1271 1271 1294	D313 1314 D348 D348 D387 D387 D387 D387 D387 D387 D387 D38
SER GLY GLY ASN ASN ASN ASN GLY GLY ASC ASC ASC ASC ASC ASC ASC ASC ASC ASC	PRU ALA CLU ARG ARG CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	L506 L506 L510 R513 R513 R513 R513 R513 R513 R515 R515
K655 K655 K559 L566 K51 E575 C588 K591 K591 L593 L595 L595	A601 L616 V619 V619 V625 D627 D627 D627 D627 D627 D627 D627 D627	GLU GLU GLY GLY GLY FRIO FRIO ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN
ASP PRO VAL PRO GLY GLY GLY GLU GLU GLU GLU GLU GLU GLZ GLZ GLZ GSG SSB SSB SSB SSB SSB SSB SSB SSB SSB	1/18 M721 F728 F728 F729 F730 L739 F739 F745 F745 F745 F746 F746 F746 F746	Y758 F756 W766 W766 W797 T825 M811 A825 L825 L825 M829 W830 W830 W830 W830
1841 1842 1843 1844 1854 1850 1855 1855 1855 1855 1855 1855 1855	1871 A872 <b>7873</b> 6874 6874 6874 6874 6874 6874 1889 1889 18895 18895 18895 18895 18895 18991 18900 19900	1903 1908 1914 1914 1926 1928 1928 1938 1938
V951 L965 1965 1967 L966 L966 1965 V971 V976 V976	1999 1990 1991 11001 11004 11006 11006 11006 11006 11006 11006 11006 11006 11006 11006 11007 111R	L1028 N1044 048 04048 04049 E1062 E1062 R1067 R1067 A1067 A1092 A14 A1092 A14 A14 A14 A14 A14 A14 A14 A14 A14 A14



#### VAL TYRE CONSTITUES CONSTITUES SERVICE SERVICE CONSTICE CONSTITUES SERVICE CONSTITUES CO

#### LYS LEU PRO PHE ILE ASP HIS

 $\bullet$  Molecule 1: Transient receptor potential melastatin 5





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32000	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	49.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, YUV, YUY

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).

Mal	Chain	Bond	lengths	Bond angles	
	Moi Chain		# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/7763	0.44	0/10588
1	В	0.25	0/7763	0.44	0/10588
1	С	0.25	0/7763	0.44	0/10588
1	D	0.25	0/7763	0.44	0/10588
All	All	0.25	0/31052	0.44	0/42352

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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	А	7574	0	7394	119	0
1	В	7574	0	7394	116	0
1	С	7574	0	7394	118	0
1	D	7574	0	7394	114	0
2	А	14	0	13	0	0
2	В	14	0	13	0	0
2	С	14	0	13	0	0
2	D	14	0	13	0	0
3	A	30	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	30	0	0	0	0
3	С	30	0	0	0	0
3	D	30	0	0	0	0
4	А	59	0	0	1	0
4	В	59	0	0	1	0
4	С	59	0	0	1	0
4	D	59	0	0	1	0
All	All	30708	0	29628	438	0

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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 7.

The worst 5 of 438 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:B:760:TRP:CZ3	1:B:1004:PRO:HD3	1.77	1.19
1:D:760:TRP:CZ3	1:D:1004:PRO:HD3	1.77	1.19
1:A:760:TRP:CZ3	1:A:1004:PRO:HD3	1.77	1.18
1:C:760:TRP:CZ3	1:C:1004:PRO:HD3	1.77	1.16
1:A:760:TRP:CZ3	1:A:1004:PRO:CD	2.58	0.86

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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	Perce	ntiles
1	А	986/1165~(85%)	958~(97%)	27 (3%)	1 (0%)	51	51
1	В	986/1165~(85%)	958~(97%)	27 (3%)	1 (0%)	51	51
1	С	986/1165~(85%)	958~(97%)	27 (3%)	1 (0%)	51	51
1	D	986/1165~(85%)	957 (97%)	28 (3%)	1 (0%)	51	51



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3944/4660~(85%)	3831~(97%)	109 (3%)	4 (0%)	54 51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1006	ILE
1	В	1006	ILE
1	С	1006	ILE
1	D	1006	ILE

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Percentile	es
1	А	743/1018~(73%)	741 (100%)	2(0%)	92 92	
1	В	743/1018~(73%)	741 (100%)	2 (0%)	92 92	
1	$\mathbf{C}$	743/1018~(73%)	741 (100%)	2(0%)	92 92	
1	D	743/1018~(73%)	741 (100%)	2(0%)	92 92	
All	All	2972/4072~(73%)	2964 (100%)	8 (0%)	92 92	

5 of 8 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	D	921	ASN
1	D	811	ARG
1	С	811	ARG
1	В	921	ASN
1	С	921	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such side chains are listed below:

1 C $514$ GLN	Mol	Chain	Res	Type
	1	С	514	GLN



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Mol	Chain	Res	Type
1	D	943	ASN
1	С	794	ASN
1	D	1010	HIS
1	D	514	GLN

#### 5.3.3 RNA (i)

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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	ol Type Chain Bes Lin		Link	Bo	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	NAG	В	1501	1	14,14,15	0.30	0	$17,\!19,\!21$	0.73	0
3	YUV	А	1502	-	35,35,35	0.12	0	$58,\!58,\!58$	0.18	0
4	YUY	С	1503	-	66,66,66	0.13	0	100,102,102	0.21	0
3	YUV	В	1502	-	35,35,35	0.12	0	$58,\!58,\!58$	0.19	0
2	NAG	С	1501	1	14,14,15	0.31	0	17,19,21	0.74	0
3	YUV	D	3003	-	35,35,35	0.13	0	$58,\!58,\!58$	0.18	0
4	YUY	D	3001	-	66,66,66	0.13	0	100,102,102	0.21	0
2	NAG	D	3002	1	14,14,15	0.31	0	17,19,21	0.73	0
4	YUY	В	1503	-	66,66,66	0.13	0	100,102,102	0.21	0
3	YUV	С	1502	-	35,35,35	0.11	0	58, 58, 58	0.19	0



Mol Tuno Chain		Chain	Chain Dog		Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	А	1501	1	14,14,15	0.29	0	17,19,21	0.75	0
4	YUY	А	1503	-	66,66,66	0.13	0	100,102,102	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	1501	1	-	1/6/23/26	0/1/1/1
3	YUV	А	1502	-	-	-	0/6/6/6
4	YUY	С	1503	-	-	16/21/149/149	0/8/8/8
3	YUV	В	1502	-	-	-	0/6/6/6
2	NAG	С	1501	1	-	1/6/23/26	0/1/1/1
4	YUY	D	3001	-	-	16/21/149/149	0/8/8/8
3	YUV	D	3003	-	-	-	0/6/6/6
2	NAG	D	3002	1	-	1/6/23/26	0/1/1/1
4	YUY	В	1503	-	-	16/21/149/149	0/8/8/8
3	YUV	С	1502	-	-	-	0/6/6/6
2	NAG	A	1501	1	-	1/6/23/26	0/1/1/1
4	YUY	А	1503	-	-	16/21/149/149	0/8/8/8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
4	А	1503	YUY	C43-C29-C30-O3
4	А	1503	YUY	C28-C29-C43-O14
4	В	1503	YUY	C43-C29-C30-O3
4	В	1503	YUY	C28-C29-C43-O14
4	С	1503	YUY	C43-C29-C30-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	1503	YUY	1	0
4	D	3001	YUY	1	0



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Mol	Chain	$\mathbf{Res}$	Type	Clashes	Symm-Clashes
4	В	1503	YUY	1	0
4	А	1503	YUY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.























### 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.



## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23744. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

#### 6.1 Orthogonal projections (i)

This section was not generated.

#### 6.2 Central slices (i)

This section was not generated.

#### 6.3 Largest variance slices (i)

This section was not generated.

### 6.4 Orthogonal surface views (i)

This section was not generated.

#### 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution (i)

This section was not generated.

#### 7.2 Volume estimate versus contour level (i)

This section was not generated.

### 7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



# 9 Map-model fit (i)

This section was not generated.

