



wwPDB EM Validation Summary Report ⓘ

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PDB ID : 9UTA / pdb_00009uta
EMDB ID : EMD-64486
Title : The transmembrane domains of human sweet taste receptor TAS1R2 and TAS1R3 in the apo state
Authors : Shi, Z.J.; Xu, W.X.; Yue, X.L.; Wu, L.J.; Hua, T.; Liu, Z.J.
Deposited on : 2025-05-03
Resolution : 3.77 Å(reported)

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

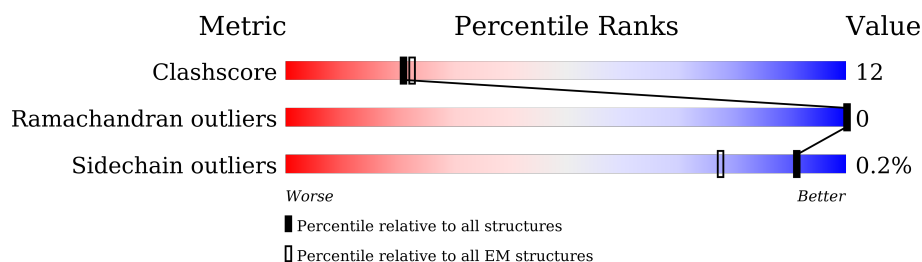
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.77 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1078	
2	B	1130	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4701 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 Taste receptor type 1 member 2, Engineered red fluorescent protein mScarlet3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	316	Total	C	N	O	S	0	0
			2487	1638	387	436	26		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP Q8TE23
A	-2	LYS	-	expression tag	UNP Q8TE23
A	-1	THR	-	expression tag	UNP Q8TE23
A	0	ILE	-	expression tag	UNP Q8TE23
A	1	ILE	-	expression tag	UNP Q8TE23
A	2	ALA	-	expression tag	UNP Q8TE23
A	3	LEU	-	expression tag	UNP Q8TE23
A	4	SER	-	expression tag	UNP Q8TE23
A	5	TYR	-	expression tag	UNP Q8TE23
A	6	ILE	-	expression tag	UNP Q8TE23
A	7	PHE	-	expression tag	UNP Q8TE23
A	8	CYS	-	expression tag	UNP Q8TE23
A	9	LEU	-	expression tag	UNP Q8TE23
A	10	VAL	-	expression tag	UNP Q8TE23
A	11	PHE	-	expression tag	UNP Q8TE23
A	12	ALA	-	expression tag	UNP Q8TE23
A	13	GLY	-	expression tag	UNP Q8TE23
A	14	SER	-	expression tag	UNP Q8TE23
A	15	ASP	-	expression tag	UNP Q8TE23
A	16	TYR	-	expression tag	UNP Q8TE23
A	17	LYS	-	expression tag	UNP Q8TE23
A	18	ASP	-	expression tag	UNP Q8TE23
A	19	ASP	-	expression tag	UNP Q8TE23
A	20	ASP	-	expression tag	UNP Q8TE23
A	21	ASP	-	expression tag	UNP Q8TE23
A	22	LYS	-	expression tag	UNP Q8TE23
A	23	GLY	-	expression tag	UNP Q8TE23

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP Q8TE23
A	25	ALA	-	expression tag	UNP Q8TE23

- Molecule 2 is a protein called Taste receptor type 1 member 3,mNeonGreen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	286	Total	C	N	O	S	0	0
			2214	1458	377	360	19		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q7RTX0
B	-6	LYS	-	expression tag	UNP Q7RTX0
B	-5	THR	-	expression tag	UNP Q7RTX0
B	-4	ILE	-	expression tag	UNP Q7RTX0
B	-3	ILE	-	expression tag	UNP Q7RTX0
B	-2	ALA	-	expression tag	UNP Q7RTX0
B	-1	LEU	-	expression tag	UNP Q7RTX0
B	0	SER	-	expression tag	UNP Q7RTX0
B	1	TYR	-	expression tag	UNP Q7RTX0
B	2	ILE	-	expression tag	UNP Q7RTX0
B	3	PHE	-	expression tag	UNP Q7RTX0
B	4	CYS	-	expression tag	UNP Q7RTX0
B	5	LEU	-	expression tag	UNP Q7RTX0
B	6	VAL	-	expression tag	UNP Q7RTX0
B	7	PHE	-	expression tag	UNP Q7RTX0
B	8	ALA	-	expression tag	UNP Q7RTX0
B	9	GLY	-	expression tag	UNP Q7RTX0
B	10	SER	-	expression tag	UNP Q7RTX0
B	11	ASP	-	expression tag	UNP Q7RTX0
B	12	TYR	-	expression tag	UNP Q7RTX0
B	13	LYS	-	expression tag	UNP Q7RTX0
B	14	ASP	-	expression tag	UNP Q7RTX0
B	15	ASP	-	expression tag	UNP Q7RTX0
B	16	ASP	-	expression tag	UNP Q7RTX0
B	17	ASP	-	expression tag	UNP Q7RTX0
B	18	LYS	-	expression tag	UNP Q7RTX0
B	19	GLY	-	expression tag	UNP Q7RTX0
B	20	SER	-	expression tag	UNP Q7RTX0
B	853	GLY	-	linker	UNP Q7RTX0
B	854	SER	-	linker	UNP Q7RTX0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	855	SER	-	linker	UNP Q7RTX0
B	856	GLY	-	linker	UNP Q7RTX0
B	857	LEU	-	linker	UNP Q7RTX0
B	858	GLU	-	linker	UNP Q7RTX0
B	859	VAL	-	linker	UNP Q7RTX0
B	860	LEU	-	linker	UNP Q7RTX0
B	861	PHE	-	linker	UNP Q7RTX0
B	862	GLN	-	linker	UNP Q7RTX0
B	863	GLY	-	linker	UNP Q7RTX0
B	864	PRO	-	linker	UNP Q7RTX0
B	865	SER	-	linker	UNP Q7RTX0
B	866	GLY	-	linker	UNP Q7RTX0
B	867	GLY	-	linker	UNP Q7RTX0
B	1103	GLY	-	expression tag	UNP A0A1S4NYF2
B	1104	SER	-	expression tag	UNP A0A1S4NYF2
B	1105	GLU	-	expression tag	UNP A0A1S4NYF2
B	1106	ASN	-	expression tag	UNP A0A1S4NYF2
B	1107	LEU	-	expression tag	UNP A0A1S4NYF2
B	1108	TYR	-	expression tag	UNP A0A1S4NYF2
B	1109	PHE	-	expression tag	UNP A0A1S4NYF2
B	1110	GLN	-	expression tag	UNP A0A1S4NYF2
B	1111	SER	-	expression tag	UNP A0A1S4NYF2
B	1112	SER	-	expression tag	UNP A0A1S4NYF2
B	1113	GLY	-	expression tag	UNP A0A1S4NYF2
B	1114	HIS	-	expression tag	UNP A0A1S4NYF2
B	1115	HIS	-	expression tag	UNP A0A1S4NYF2
B	1116	HIS	-	expression tag	UNP A0A1S4NYF2
B	1117	HIS	-	expression tag	UNP A0A1S4NYF2
B	1118	HIS	-	expression tag	UNP A0A1S4NYF2
B	1119	HIS	-	expression tag	UNP A0A1S4NYF2
B	1120	HIS	-	expression tag	UNP A0A1S4NYF2
B	1121	HIS	-	expression tag	UNP A0A1S4NYF2
B	1122	HIS	-	expression tag	UNP A0A1S4NYF2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70080	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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	0.24	0/2556	0.40	0/3489
2	B	0.27	0/2278	0.45	1/3118 (0.0%)
All	All	0.26	0/4834	0.43	1/6607 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	791	PRO	CA-N-CD	-8.94	99.49	112.00

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	A	2487	0	2506	60	0
2	B	2214	0	2275	51	0
All	All	4701	0	4781	111	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 12.

The worst 5 of 111 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:A:638:PRO:O	1:A:689:LYS:NZ	2.21	0.70
1:A:660:LYS:O	1:A:664:ARG:N	2.29	0.65
1:A:615:TYR:OH	1:A:801:LEU:HD23	1.97	0.65
1:A:560:GLU:OE1	1:A:561:TRP:N	2.27	0.65
1:A:786:VAL:HG12	1:A:786:VAL:O	1.95	0.65

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	Percentiles	
1	A	314/1078 (29%)	277 (88%)	37 (12%)	0	100	100
2	B	284/1130 (25%)	266 (94%)	18 (6%)	0	100	100
All	All	598/2208 (27%)	543 (91%)	55 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	281/955 (29%)	281 (100%)	0	100	100
2	B	238/941 (25%)	237 (100%)	1 (0%)	89	93
All	All	519/1896 (27%)	518 (100%)	1 (0%)	91	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	699	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	637	GLN
2	B	712	HIS
2	B	734	HIS

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 oligosaccharides 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.