



Full wwPDB EM Validation Report ⓘ

Apr 26, 2026 – 12:21 AM JST

PDB ID : 9W0R / pdb_00009w0r
EMDB ID : EMD-65513
Title : Cryo-EM structure of apo-T2R46 in complex with heterotrimeric G protein
Authors : Tan, Q.; Yu, Y.; Han, X.; Zhao, Q.; Wu, B.
Deposited on : 2025-07-24
Resolution : 2.70 Å (reported)
Based on initial model : 7x9a

This is a Full wwPDB EM Validation 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 Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

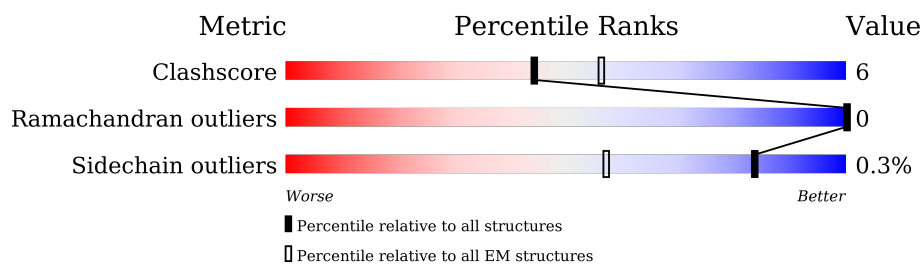
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	R	363	
2	A	354	
3	B	351	
4	C	71	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6650 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 2 member 46.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	271	Total	C	N	O	S	0	0
			2086	1399	337	340	10		

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-21	MET	-	initiating methionine	UNP P59540
R	-20	LYS	-	expression tag	UNP P59540
R	-19	THR	-	expression tag	UNP P59540
R	-18	ILE	-	expression tag	UNP P59540
R	-17	ILE	-	expression tag	UNP P59540
R	-16	ALA	-	expression tag	UNP P59540
R	-15	LEU	-	expression tag	UNP P59540
R	-14	SER	-	expression tag	UNP P59540
R	-13	TYR	-	expression tag	UNP P59540
R	-12	ILE	-	expression tag	UNP P59540
R	-11	PHE	-	expression tag	UNP P59540
R	-10	CYS	-	expression tag	UNP P59540
R	-9	LEU	-	expression tag	UNP P59540
R	-8	VAL	-	expression tag	UNP P59540
R	-7	PHE	-	expression tag	UNP P59540
R	-6	ALA	-	expression tag	UNP P59540
R	-5	ASP	-	expression tag	UNP P59540
R	-4	TYR	-	expression tag	UNP P59540
R	-3	LYS	-	expression tag	UNP P59540
R	-2	ASP	-	expression tag	UNP P59540
R	-1	ASP	-	expression tag	UNP P59540
R	0	ASP	-	expression tag	UNP P59540
R	305	PHE	-	expression tag	UNP P59540
R	306	LEU	-	expression tag	UNP P59540
R	307	GLU	-	expression tag	UNP P59540
R	308	VAL	-	expression tag	UNP P59540
R	309	LEU	-	expression tag	UNP P59540
R	310	PHE	-	expression tag	UNP P59540

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	311	GLN	-	expression tag	UNP P59540
R	312	GLY	-	expression tag	UNP P59540
R	313	PRO	-	expression tag	UNP P59540
R	314	TRP	-	expression tag	UNP P59540
R	315	SER	-	expression tag	UNP P59540
R	316	HIS	-	expression tag	UNP P59540
R	317	PRO	-	expression tag	UNP P59540
R	318	GLN	-	expression tag	UNP P59540
R	319	PHE	-	expression tag	UNP P59540
R	320	GLU	-	expression tag	UNP P59540
R	321	LYS	-	expression tag	UNP P59540
R	322	GLY	-	expression tag	UNP P59540
R	323	GLY	-	expression tag	UNP P59540
R	324	GLY	-	expression tag	UNP P59540
R	325	SER	-	expression tag	UNP P59540
R	326	GLY	-	expression tag	UNP P59540
R	327	GLY	-	expression tag	UNP P59540
R	328	GLY	-	expression tag	UNP P59540
R	329	SER	-	expression tag	UNP P59540
R	330	GLY	-	expression tag	UNP P59540
R	331	GLY	-	expression tag	UNP P59540
R	332	SER	-	expression tag	UNP P59540
R	333	ALA	-	expression tag	UNP P59540
R	334	TRP	-	expression tag	UNP P59540
R	335	SER	-	expression tag	UNP P59540
R	336	HIS	-	expression tag	UNP P59540
R	337	PRO	-	expression tag	UNP P59540
R	338	GLN	-	expression tag	UNP P59540
R	339	PHE	-	expression tag	UNP P59540
R	340	GLU	-	expression tag	UNP P59540
R	341	LYS	-	expression tag	UNP P59540

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	215	Total	C	N	O	S	0	0
			1673	1070	287	304	12		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	THR	GLY	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

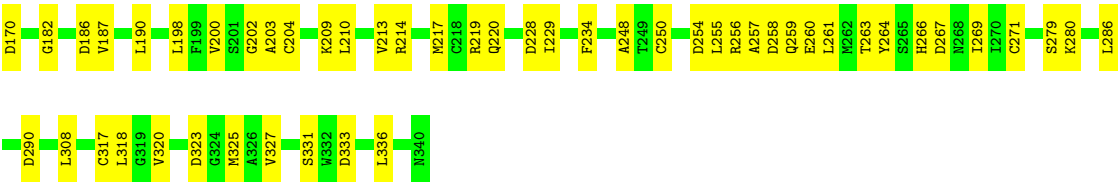
Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	334	Total	C	N	O	S	0	0
			2506	1553	445	487	21		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	54	Total	C	N	O	S	0	0
			385	244	67	71	3		



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1968661	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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	R	0.12	0/2137	0.36	0/2920
2	A	0.08	0/1702	0.23	0/2288
3	B	0.09	0/2553	0.28	0/3470
4	C	0.10	0/391	0.31	0/534
All	All	0.10	0/6783	0.30	0/9212

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	R	2086	0	2121	30	0
2	A	1673	0	1626	13	0
3	B	2506	0	2378	43	0
4	C	385	0	371	6	0
All	All	6650	0	6496	84	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 6.

All (84) 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)
3:B:286:LEU:HB3	3:B:318:LEU:HD21	1.68	0.75
3:B:254:ASP:HB2	3:B:261:LEU:HD11	1.73	0.71
3:B:325:MET:HE2	4:C:60:PRO:HD2	1.73	0.70
1:R:108:LEU:O	1:R:122:LYS:NZ	2.27	0.64
3:B:104:ALA:HB3	3:B:113:ALA:HB3	1.79	0.64
1:R:223:VAL:HG21	2:A:345:LYS:HE2	1.79	0.63
1:R:233:SER:HB3	1:R:278:ILE:HD11	1.81	0.63
2:A:251:ASP:OD1	2:A:255:ASN:ND2	2.32	0.62
3:B:320:VAL:HG22	3:B:327:VAL:HG22	1.80	0.61
1:R:17:PHE:O	1:R:21:ASN:ND2	2.33	0.61
2:A:209:LYS:NZ	3:B:228:ASP:OD2	2.32	0.61
2:A:184:ILE:HD11	2:A:199:PHE:HB3	1.83	0.60
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.84	0.59
3:B:51:LEU:HB2	3:B:336:LEU:HB2	1.84	0.59
1:R:71:LEU:HG	1:R:73:PRO:HD3	1.84	0.59
3:B:158:VAL:HG12	3:B:190:LEU:HD11	1.85	0.58
3:B:45:MET:HE3	3:B:308:LEU:HD21	1.85	0.58
1:R:17:PHE:CD1	1:R:63:VAL:HG21	2.39	0.57
3:B:149:CYS:O	3:B:150:ARG:NH1	2.37	0.57
3:B:79:LEU:HD22	3:B:95:LEU:HD21	1.87	0.56
3:B:145:TYR:O	3:B:162:GLY:N	2.35	0.56
3:B:198:LEU:HD12	3:B:210:LEU:HD11	1.87	0.55
3:B:325:MET:HE1	4:C:54:VAL:HG21	1.89	0.54
2:A:36:LEU:HD12	2:A:198:MET:HG2	1.89	0.54
3:B:331:SER:OG	3:B:333:ASP:OD1	2.26	0.54
1:R:145:PHE:O	1:R:149:MET:HG3	2.08	0.54
2:A:229:ASP:HB2	2:A:286:CYS:HB2	1.90	0.54
3:B:186:ASP:H	3:B:204:CYS:HB2	1.74	0.53
1:R:204:LYS:HA	1:R:207:LYS:HE2	1.90	0.53
3:B:260:GLU:OE2	3:B:263:THR:OG1	2.28	0.52
3:B:155:ASN:ND2	3:B:170:ASP:OD1	2.43	0.51
3:B:78:LYS:HD3	3:B:94:PRO:HA	1.93	0.51
1:R:280:ILE:HG22	1:R:286:LEU:HD13	1.93	0.50
1:R:177:THR:HB	1:R:179:VAL:HG22	1.94	0.50
3:B:254:ASP:HB3	3:B:257:ALA:HB3	1.94	0.49
2:A:325:CYS:SG	2:A:326:SER:N	2.85	0.49
3:B:168:LEU:HD22	3:B:213:VAL:HG13	1.94	0.49
1:R:59:LEU:O	1:R:63:VAL:HG23	2.13	0.49
3:B:220:GLN:NE2	3:B:258:ASP:OD1	2.46	0.49
1:R:17:PHE:CE1	1:R:63:VAL:HG21	2.48	0.48
1:R:53:VAL:HA	1:R:56:VAL:HG22	1.96	0.48
2:A:35:LYS:HB3	2:A:218:VAL:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:187:VAL:HA	3:B:203:ALA:HA	1.96	0.47
2:A:241:ASN:HD22	2:A:242:ARG:H	1.63	0.47
3:B:256:ARG:HB3	4:C:28:ILE:HG12	1.96	0.47
4:C:13:ARG:HA	4:C:16:VAL:HG22	1.96	0.47
1:R:298:ARG:HA	1:R:301:VAL:HG12	1.96	0.47
3:B:248:ALA:HB1	3:B:269:ILE:HG22	1.97	0.46
3:B:219:ARG:NH2	4:C:21:MET:HE1	2.30	0.46
1:R:237:LEU:HD13	1:R:278:ILE:HG21	1.98	0.46
1:R:35:TRP:HE3	1:R:41:ILE:HG12	1.80	0.45
1:R:223:VAL:HG23	1:R:224:HIS:CD2	2.51	0.45
3:B:217:MET:SD	3:B:219:ARG:NH2	2.90	0.45
1:R:216:SER:HA	1:R:220:SER:HB3	1.98	0.45
1:R:96:ASN:ND2	1:R:184:ASN:OD1	2.50	0.44
3:B:182:GLY:O	3:B:209:LYS:HE3	2.17	0.44
3:B:213:VAL:HG12	3:B:214:ARG:HD2	1.99	0.44
3:B:124:TYR:CE1	3:B:135:VAL:HG22	2.52	0.44
3:B:93:ILE:HG12	3:B:133:VAL:HG11	2.00	0.44
3:B:200:VAL:HG22	3:B:234:PHE:CE2	2.53	0.44
1:R:34:GLU:HA	1:R:37:LYS:HB3	2.00	0.43
1:R:205:HIS:NE2	2:A:341:ASP:OD1	2.42	0.43
3:B:250:CYS:HB2	3:B:264:TYR:HB2	2.01	0.43
3:B:202:GLY:HA3	3:B:229:ILE:HG21	1.99	0.43
1:R:43:PHE:CE2	1:R:47:ILE:HD11	2.54	0.42
1:R:281:TRP:HA	1:R:287:LYS:HE3	2.01	0.42
2:A:241:ASN:HD22	2:A:242:ARG:N	2.17	0.42
1:R:128:VAL:O	1:R:132:ILE:HG12	2.18	0.42
3:B:210:LEU:HD22	3:B:255:LEU:HD22	2.01	0.42
1:R:115:ASN:O	1:R:119:LEU:HG	2.20	0.42
1:R:138:LEU:HA	1:R:141:VAL:HG12	2.02	0.42
3:B:146:LEU:HA	3:B:161:SER:HA	2.01	0.42
2:A:21:ARG:HG2	2:A:24:ARG:HH22	1.85	0.41
3:B:279:SER:HB2	4:C:50:LEU:HD12	2.02	0.41
3:B:156:GLN:HB3	3:B:168:LEU:HD11	2.03	0.41
1:R:218:ASP:HB3	1:R:219:PRO:HD3	2.02	0.41
1:R:62:LEU:HD21	1:R:269:PHE:CZ	2.56	0.41
1:R:112:ASN:O	1:R:112:ASN:ND2	2.42	0.41
3:B:51:LEU:HB3	3:B:82:TRP:CE3	2.56	0.41
3:B:280:LYS:HD2	3:B:323:ASP:O	2.20	0.41
3:B:61:MET:HG3	3:B:317:CYS:HB2	2.03	0.41
2:A:34:VAL:HG13	2:A:219:THR:HG21	2.03	0.40
1:R:144:LEU:HA	1:R:147:ILE:HD13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:266:HIS:CD2	3:B:267:ASP:H	2.39	0.40

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	R	265/363 (73%)	252 (95%)	13 (5%)	0	100	100
2	A	209/354 (59%)	207 (99%)	2 (1%)	0	100	100
3	B	332/351 (95%)	324 (98%)	8 (2%)	0	100	100
4	C	52/71 (73%)	52 (100%)	0	0	100	100
All	All	858/1139 (75%)	835 (97%)	23 (3%)	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	R	220/325 (68%)	219 (100%)	1 (0%)	81	92
2	A	172/306 (56%)	172 (100%)	0	100	100
3	B	263/293 (90%)	262 (100%)	1 (0%)	84	93
4	C	36/58 (62%)	36 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	691/982 (70%)	689 (100%)	2 (0%)	84	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	112	ASN
3	B	259	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	21	ASN
1	R	24	ASN
1	R	86	ASN
1	R	92	ASN
1	R	96	ASN
2	A	47	ASN
2	A	195	HIS
2	A	241	ASN
2	A	294	ASN
3	B	142	HIS
3	B	155	ASN
3	B	183	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.