



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:02 AM UTC

PDB ID : 7X1T / pdb_00007x1t
EMDB ID : EMD-32949
Title : Structure of Thyrotropin-Releasing Hormone Receptor bound with Taltirelin.
Authors : Yang, F.; Zhang, H.H.; Meng, X.Y.; Li, Y.G.; Zhou, Y.X.; Ling, S.L.; Liu, L.;
Shi, P.; Tian, C.L.
Deposited on : 2022-02-24
Resolution : 3.26 Å(reported)

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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

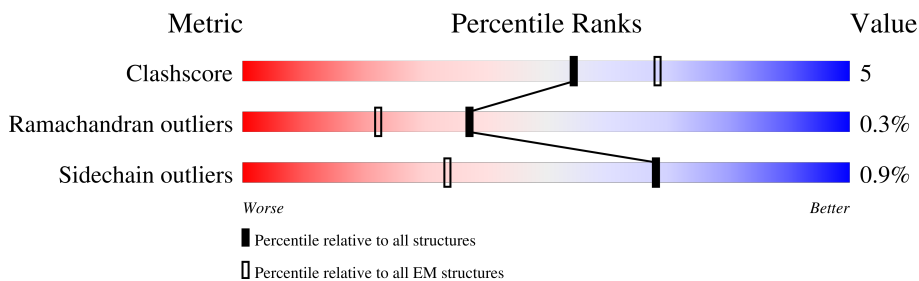
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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	F	71	
2	A	398	
3	B	246	
4	C	340	
5	D	251	
6	E	5	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7488 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 Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	49	Total	C	N	O	S	0	0
			299	190	52	55	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	68	SER	CYS	conflict	UNP P63212

- Molecule 2 is a protein called Thyrotropin-releasing hormone receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	272	Total	C	N	O	S	0	0
			1958	1301	318	327	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	LEU	ILE	conflict	UNP P34981

- Molecule 3 is a protein called mini-G alpha q protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	218	Total	C	N	O	S	0	0
			1578	1010	280	282	6		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

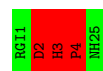
Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	330	Total	C	N	O	S	0	0
			2288	1436	393	441	18		

- Molecule 5 is a protein called ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	209	Total	C	N	O	S	0	0
			1336	836	232	263	5		

- Molecule 6 is a protein called Taltirelin.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	5	Total	C	N	O	0	1
			29	17	7	5		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	394270	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RGI, NH2

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	F	0.15	0/304	0.36	0/423
2	A	0.22	0/1998	0.62	0/2741
3	B	0.20	0/1604	0.49	0/2181
4	C	0.22	0/2331	0.50	0/3193
5	D	0.25	0/1361	0.66	0/1870
6	E	4.38	6/25 (24.0%)	2.48	2/33 (6.1%)
All	All	0.33	6/7623 (0.1%)	0.57	2/10441 (0.0%)

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
2	A	0	1
6	E	2	0
All	All	2	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	3	HIS	C-N	9.45	1.49	1.34
6	E	4	PRO	N-CD	-8.67	1.35	1.47
6	E	2	ASP	C-N	7.45	1.49	1.33
6	E	3	HIS	CA-C	6.62	1.61	1.52
6	E	3	HIS	C-O	-6.16	1.16	1.24
6	E	4	PRO	N-CA	5.24	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	2	ASP	CA-CB-CG	6.93	119.53	112.60
6	E	2	ASP	N-CA-CB	5.60	120.02	110.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	3	HIS	CA
6	E	4	PRO	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	80	LEU	Peptide

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	F	299	0	243	1	0
2	A	1958	0	1881	9	0
3	B	1578	0	1421	19	0
4	C	2288	0	2040	33	0
5	D	1336	0	1043	14	0
6	E	29	0	20	1	0
All	All	7488	0	6648	72	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 5.

All (72) 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)
2:A:123:ARG:NH1	2:A:211:TYR:OH	2.31	0.63
5:D:63:THR:HG23	5:D:64:VAL:HG23	1.81	0.62
4:C:320:VAL:HG22	4:C:327:VAL:HG22	1.86	0.58
4:C:157:ILE:HG23	4:C:169:TRP:HB2	1.86	0.57
3:B:19:ILE:HG23	4:C:92:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:276:VAL:HG13	4:C:285:LEU:HD11	1.87	0.56
5:D:8:GLY:HA3	5:D:20:LEU:HD22	1.87	0.56
4:C:79:LEU:HB3	4:C:93:ILE:HB	1.87	0.56
5:D:6:GLU:HA	5:D:22:CYS:HA	1.87	0.55
5:D:22:CYS:SG	5:D:23:SER:N	2.78	0.55
4:C:129:ARG:O	5:D:2:VAL:N	2.39	0.55
3:B:216:THR:OG1	3:B:226:ARG:NH2	2.40	0.54
5:D:175:LEU:HD21	5:D:178:TYR:HB3	1.89	0.54
4:C:211:TRP:HA	4:C:218:CYS:HA	1.90	0.54
1:F:51:LEU:HD21	4:C:283:ARG:HB3	1.89	0.54
4:C:166:CYS:HB2	4:C:180:PHE:HB2	1.91	0.51
3:B:106:ILE:HD11	3:B:134:LEU:HD22	1.93	0.51
4:C:290:ASP:OD1	4:C:314:ARG:NE	2.41	0.51
3:B:143:LEU:HD21	3:B:197:PHE:HE2	1.76	0.50
4:C:165:THR:HG22	4:C:181:THR:HG22	1.94	0.50
3:B:69:ILE:HG13	4:C:117:LEU:HB3	1.94	0.49
4:C:187:VAL:HA	4:C:203:ALA:HA	1.93	0.48
2:A:146:ILE:HA	2:A:149:VAL:HG12	1.96	0.48
4:C:145:TYR:O	4:C:162:GLY:N	2.46	0.48
4:C:121:CYS:HB3	4:C:139:LEU:HB2	1.95	0.48
3:B:22:ASN:ND2	3:B:25:GLU:OE2	2.47	0.47
5:D:62:ASP:N	5:D:62:ASP:OD1	2.47	0.47
4:C:192:LEU:HD23	4:C:199:PHE:HB3	1.96	0.47
4:C:275:SER:OG	4:C:316:SER:O	2.33	0.47
2:A:113:SER:OG	2:A:199:PHE:O	2.32	0.46
3:B:35:ARG:HB2	3:B:103:VAL:HG23	1.98	0.46
4:C:222:PHE:HE1	4:C:258:ASP:HA	1.80	0.46
3:B:239:ASN:HA	3:B:242:GLU:HB3	1.98	0.45
3:B:112:SER:HA	3:B:118:LEU:HD21	1.98	0.45
2:A:105:GLN:HB3	6:E:4:PRO:HB2	1.97	0.45
3:B:69:ILE:HD12	3:B:86:VAL:HG13	1.98	0.44
3:B:153:VAL:HG11	3:B:186:VAL:HB	2.00	0.44
4:C:58:ILE:O	4:C:316:SER:OG	2.25	0.44
3:B:103:VAL:HG12	3:B:137:ILE:HD13	1.98	0.44
4:C:227:SER:OG	4:C:228:ASP:N	2.45	0.44
4:C:163:ASP:N	4:C:163:ASP:OD1	2.50	0.44
2:A:209:VAL:HG12	2:A:210:LEU:HD23	1.98	0.44
5:D:161:TYR:HD2	5:D:221:LEU:HG	1.81	0.44
4:C:161:SER:OG	4:C:162:GLY:N	2.47	0.44
4:C:186:ASP:H	4:C:204:CYS:HB3	1.83	0.44
5:D:178:TYR:HD2	5:D:179:ARG:HG2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:160:SER:OG	4:C:187:VAL:O	2.36	0.44
2:A:113:SER:OG	2:A:113:SER:O	2.36	0.43
4:C:55:LEU:HD23	4:C:55:LEU:HA	1.88	0.43
4:C:230:ASN:OD1	4:C:230:ASN:N	2.52	0.43
4:C:210:LEU:O	4:C:219:ARG:N	2.52	0.43
3:B:35:ARG:HB3	3:B:84:PHE:HE2	1.84	0.43
3:B:238:MET:O	3:B:242:GLU:N	2.51	0.43
5:D:152:SER:HA	5:D:198:THR:HB	2.00	0.42
4:C:162:GLY:HA2	4:C:186:ASP:HB3	2.01	0.42
4:C:242:ALA:HA	4:C:252:LEU:HA	2.02	0.42
2:A:63:TYR:HA	2:A:146:ILE:HD11	2.02	0.42
3:B:195:LYS:HA	3:B:198:VAL:HG22	2.02	0.42
4:C:247:ASP:OD1	4:C:247:ASP:N	2.53	0.42
5:D:220:HIS:O	5:D:220:HIS:ND1	2.53	0.42
3:B:131:ASN:HD22	3:B:134:LEU:HD12	1.85	0.42
5:D:138:THR:HA	5:D:139:PRO:HD3	1.92	0.41
3:B:231:CYS:HA	3:B:234:ILE:HD12	2.03	0.41
5:D:70:ILE:HA	5:D:81:LEU:HA	2.02	0.41
4:C:83:ASP:N	4:C:88:ASN:O	2.44	0.41
4:C:271:CYS:HB3	4:C:290:ASP:HB2	2.03	0.41
3:B:214:HIS:CE1	3:B:226:ARG:HB3	2.56	0.40
5:D:7:SER:N	5:D:21:SER:O	2.54	0.40
3:B:34:LEU:HB3	3:B:104:THR:HG21	2.03	0.40
4:C:54:HIS:CE1	4:C:80:ILE:HD12	2.56	0.40
2:A:74:VAL:HB	2:A:108:GLY:HA3	2.04	0.40
2:A:97:GLY:O	2:A:101:ILE:N	2.45	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	F	47/71 (66%)	42 (89%)	5 (11%)	0	100	100
2	A	268/398 (67%)	256 (96%)	12 (4%)	0	100	100
3	B	210/246 (85%)	197 (94%)	13 (6%)	0	100	100
4	C	328/340 (96%)	299 (91%)	29 (9%)	0	100	100
5	D	199/251 (79%)	164 (82%)	35 (18%)	0	100	100
6	E	3/5 (60%)	0	0	3 (100%)	0	0
All	All	1055/1311 (80%)	958 (91%)	94 (9%)	3 (0%)	37	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	2	ASP
6	E	3	HIS
6	E	4	PRO

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	F	19/58 (33%)	19 (100%)	0	100	100
2	A	183/363 (50%)	182 (100%)	1 (0%)	81	82
3	B	139/213 (65%)	138 (99%)	1 (1%)	76	79
4	C	210/283 (74%)	208 (99%)	2 (1%)	68	75
5	D	101/201 (50%)	101 (100%)	0	100	100
6	E	3/3 (100%)	1 (33%)	2 (67%)	0	0
All	All	655/1121 (58%)	649 (99%)	6 (1%)	68	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	138	THR
3	B	76	VAL

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Mol	Chain	Res	Type
4	C	315	VAL
4	C	318	LEU
6	E	2	ASP
6	E	3	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	105	GLN
2	A	312	ASN
3	B	22	ASN
3	B	82	HIS
4	C	32	GLN
4	C	88	ASN
4	C	142	HIS
5	D	159	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	RGI	E	1	6	3,3,4	1.00	0	2,2,4	0.32	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
6	RGI	E	1	6	-	0/1/1/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32949. 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 standard-deviation projections (False-color) [i](#)

This section was not generated.

6.5 Orthogonal surface views [i](#)

This section was not generated.

6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.