



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:54 AM UTC

PDB ID : 6KR8 / pdb_00006kr8
BMRB ID : 36284
Title : Structure of the beta2 adrenergic receptor in the full agonist bound state
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Deposited on : 2019-08-21

This is a wwPDB NMR Structure 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/NMRValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

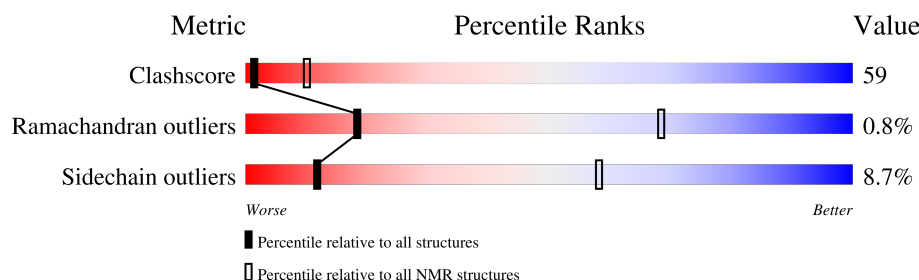
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	336	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:30-A:55, A:63-A:133, A:141-A:144, A:150-A:237, A:273-A:341 (258)	0.12	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 7, 8, 9
2	3, 10
Single-model clusters	2

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5052 atoms, of which 2544 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called beta 2 adrenergic receptor.

Mol	Chain	Residues	Atoms						Trace
1	A	312	Total	C	H	N	O	S	0
			5052	1651	2544	413	425	19	

HIS	L284	L212	A150	V86
HIS	C285	V213	R151	V87
HIS	W286	I214	I152	F88
HIS	L287	M215	I153	F89
HIS	P288	V216		G90
HIS	F289	F217	M156	A91
HIS	F290	V218	V157	A92
HIS	I291	V219	I158	H93
HIS	V292		I159	I94
	N293	F222	V160	
	I294	V223	S161	K97
	V295		G162	T98
	H296	R228	L163	A99
	V297		T164	T100
	I298	K232	S165	F101
	Q299		F166	G102
	D300	G238	L167	N103
	N301	R239	P168	F104
	L302	F240	I169	W105
	I303	H241	Q170	G106
		V242	M171	E107
	E306	Q243	H172	F108
	V307	N244	W173	W109
		V245	Y174	T110
	L310	S246	R175	S111
	L311	Q247	A176	T112
	N312	V248	T177	D113
	W313	E249	H178	W114
	I314	Q250	Q179	L115
	G315	D251	E180	C116
	Y316	G252	A181	V117
	V317	R253	I182	T118
	N318	T254	M183	
		G255	C184	W122
	F321	H256	Y185	T123
	N322	G257	A186	L124
	P323	H258	E187	C125
	L324	R259	E188	V126
	I325	R260	T189	I127
	Y326	S261	C190	A128
	S327	S262	C191	V129
	R328	K263	D192	
	S329	F264	F193	Y132
		A265	F194	F133
	C334	C266	T195	A134
	A335	K267	M196	I135
	F336	E268	Q197	C136
		H269	A198	S137
	L340	K270	Y199	P138
	A341	A271	A200	F139
ALA		L272	I201	K140
ARG			A202	Y141
ARG	L275			Q142
SER	G276	I205	I206	S143
SER	I277	V206	V206	L144
SER	L278	S207	S207	L145
VAL	K279	F208	F208	T146
LYS		Y209	Y209	K147
ALA		V210	V210	C148
HIS	F282			K149
HIS	T283		P211	

5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 500 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
X-PLOR NIH	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	38
Number of shifts mapped to atoms	38
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality [i](#)

6.1 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 (average) 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	1.32±0.00	1±0/2139 (0.0± 0.0%)	1.50±0.01	22±1/2922 (0.7± 0.0%)
All	All	1.32	10/21390 (0.0%)	1.50	218/29220 (0.7%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	210	VAL	CA-CB	-6.79	1.50	1.54	1	10

5 of 28 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	101	PHE	CA-CB-CG	-10.57	103.23	113.80	1	10
1	A	150	ALA	CA-C-N	8.71	131.95	120.28	7	1
1	A	150	ALA	C-N-CA	8.71	131.95	120.28	7	1
1	A	300	ASP	CA-CB-CG	-7.36	105.24	112.60	1	10
1	A	326	TYR	N-CA-C	7.36	120.00	111.02	2	2

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2082	2114	2106	245±6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	20820	21140	21060	2452

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 59.

5 of 333 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:285:CYS:O	1:A:286:TRP:CG	1.07	2.08	7	10
1:A:285:CYS:O	1:A:286:TRP:CD1	0.98	2.17	7	8
1:A:176:ALA:HB3	1:A:194:PHE:HE2	0.90	1.25	1	10
1:A:285:CYS:HB3	1:A:314:ILE:O	0.90	1.66	5	10
1:A:285:CYS:CB	1:A:314:ILE:O	0.88	2.21	7	10

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	256/336 (76%)	245±1 (96±0%)	9±1 (4±0%)	2±1 (1±0%)	18	68
All	All	2560/3360 (76%)	2447 (96%)	93 (4%)	20 (1%)	18	68

5 of 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	286	TRP	10
1	A	133	PHE	3
1	A	326	TYR	2
1	A	150	ALA	2
1	A	327	SER	1

6.3.2 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 NMR 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	229/296 (77%)	209±2 (91±1%)	20±2 (9±1%)	12 58
All	All	2290/2960 (77%)	2090 (91%)	200 (9%)	12 58

5 of 36 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	38	ILE	10
1	A	72	ILE	10
1	A	75	LEU	10
1	A	93	HIS	10
1	A	142	GLN	10

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *PeakList.star*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	38
Number of shifts mapped to atoms	38
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 34 atoms were assigned a chemical shift out of a possible 3695. 0 out of 56 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	34/1289 (3%)	17/521 (3%)	0/516 (0%)	17/252 (7%)
Sidechain	0/1977 (0%)	0/1317 (0%)	0/607 (0%)	0/53 (0%)
Aromatic	0/429 (0%)	0/209 (0%)	0/203 (0%)	0/17 (0%)
Overall	34/3695 (1%)	17/2047 (1%)	0/1326 (0%)	17/322 (5%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

