wwPDB NMR Structure Validation Summary Report

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PDB ID	:	6KR8
BMRB ID	:	36284
Title	:	Structure of the beta2 adrenergic receptor in the full agonist bound state
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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 (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 (i)) were used in the production of this report:

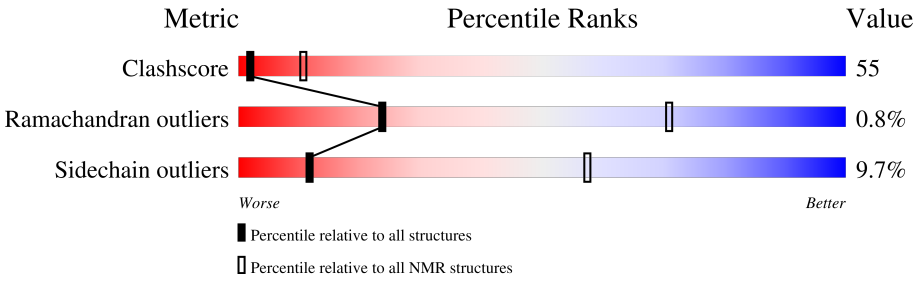
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 0%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	336	29% 45% • 16% 7%

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
			Total	C	H	N	O	S	
1	A	312	5052	1651	2544	413	425	19	0

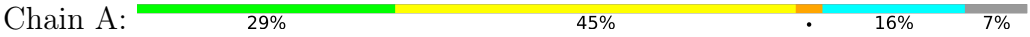
4 Residue-property plots (i)

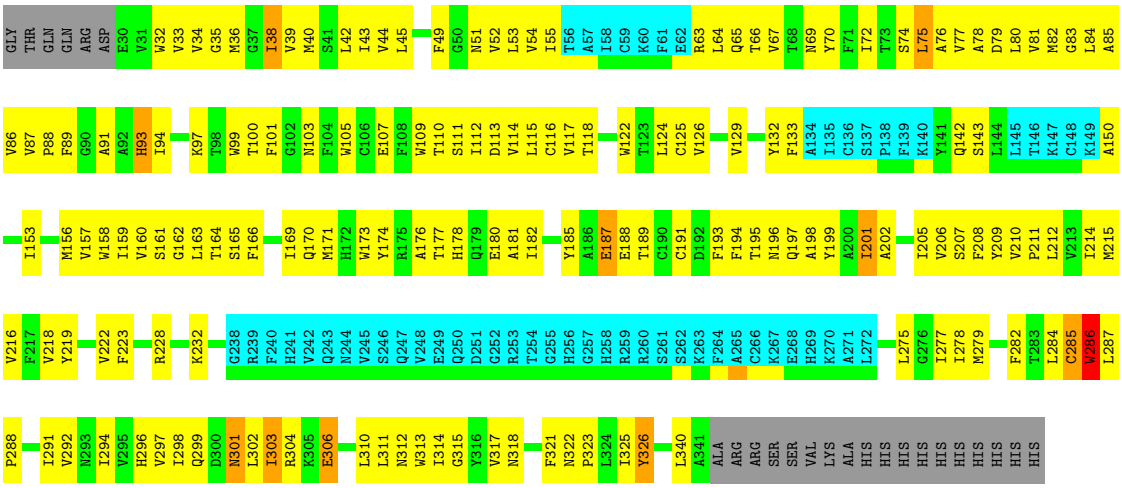
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: beta 2 adrenergic receptor

Chain A:



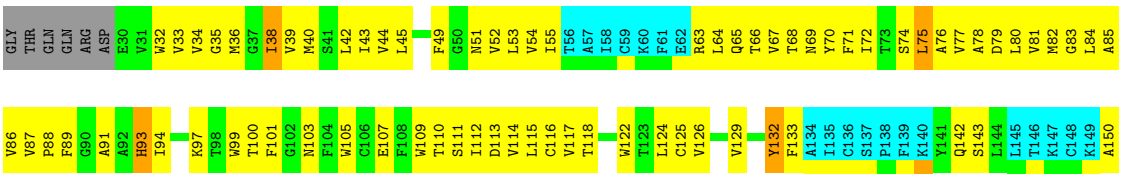


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: beta 2 adrenergic receptor

Chain A:




R151 V152 I153 M156 V157 W158 I159 V160 S161 G162 L163 T164 S165 F166 I169 Q170 M171 H172 W173 Y174 R175 A176 T177 H178 Q179 E180 A181 I182 Y185 A186 E187 E188 T189 C190 C191 D192 F193 F194 T195 N196 Q197 A198 Y199 A200 I201 A202 I205 V206 S207 F208 Y209 V210 P211 L212 V213 I214
M215 V216 F217 V218 Y219 V222 F223 R228 K232 G238 R239 F240 H241 V242 Q243 N244 V245 S246 Q247 V248 E249 Q250 D251 G252 R253 T254 G255 H256 G257 H258 R259 R260 S261 S262 K263 P264 A265 C266 K267 E268 H269 K270 A271 L272 L275 G276 I277 I278 M279 F282 T283 L284 C285 W286
L287 P288 I291 V292 N293 I294 V295 H296 V297 I298 N301 L302 I303 E306 V307 L310 L311 N312 W313 I314 G315 Y316 V317 N318 F321 N322 P323 L324 I325 Y326 L340 A341 ALA ARG ARG SER SER VAL LYS ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

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	19
Number of unparsed shifts	0
Number of shifts with mapping errors	19
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	232±6
All	All	20820	21140	21060	2323

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 55.

5 of 321 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:36:MET:HG2	1:A:40:MET:HE2	0.89	1.42	1	10

6.3 Torsion angles

6.3.1 Protein backbone

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%)	24 71
All	All	2560/3360 (76%)	2447 (96%)	93 (4%)	20 (1%)	24 71

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%)	207±2 (90±1%)	22±2 (10±1%)	12 57
All	All	2290/2960 (77%)	2067 (90%)	223 (10%)	12 57

5 of 39 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 monosaccharides 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 (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% 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

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	19
Number of unparsed shifts	0
Number of shifts with mapping errors	19
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 19) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	LEU	HN	7.96	0.02	.
1	A	45	LEU	HN	8.23	0.02	.
1	A	53	LEU	HN	8.01	0.02	.
1	A	64	LEU	HN	7.88	0.02	.
1	A	80	LEU	HN	8.9	0.02	.
1	A	84	LEU	HN	8.13	0.02	.
1	A	115	LEU	HN	8.64	0.02	.
1	A	144	LEU	HN	8.04	0.02	.
1	A	145	LEU	HN	7.61	0.02	.
1	A	155	LEU	HN	8.21	0.02	.
1	A	163	LEU	HN	8.65	0.02	.
1	A	167	LEU	HN	7.15	0.02	.
1	A	212	LEU	HN	7.95	0.02	.
1	A	230	LEU	HN	7.85	0.02	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	266	CYS	HN	8.11	0.02	.
1	A	284	LEU	HN	8.39	0.02	.
1	A	287	LEU	HN	7.81	0.02	.
1	A	311	LEU	HN	8.31	0.02	.
1	A	340	LEU	HN	7.77	0.02	.

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 0%, i.e. 17 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	17/1289 (1%)	0/521 (0%)	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	17/3695 (0%)	0/2047 (0%)	0/1326 (0%)	17/322 (5%)

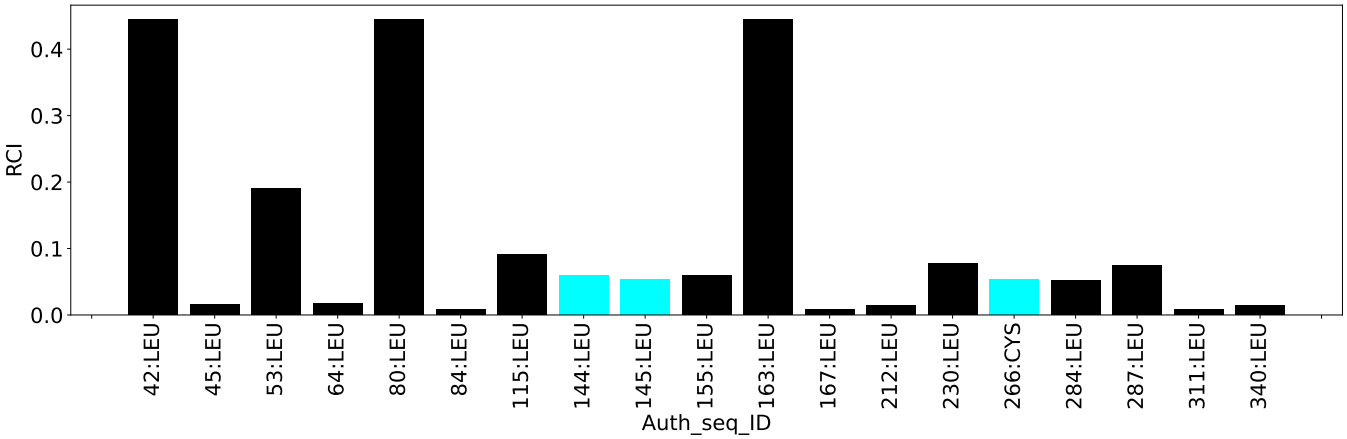
7.1.4 Statistically unusual chemical shifts (i)

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:


RCI
0.0
0.1
0.2
0.3
0.4
42:LEU
45:LEU
53:LEU
64:LEU
80:LEU
84:LEU
115:LEU
144:LEU
145:LEU
155:LEU
163:LEU
167:LEU
212:LEU
230:LEU
266:CYS
284:LEU
287:LEU
311:LEU
340:LEU
Auth_seq_ID