



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:07 PM GMT

PDB ID : 2R4R
Title : Crystal structure of the human beta2 adrenoceptor
Authors : Rasmussen, S.G.F.; Choi, H.J.; Rosenbaum, D.M.; Kobilka, T.S.; Thian, F.S.;
Edwards, P.C.; Burghammer, M.; Ratnala, V.R.; Sanishvili, R.; Fischetti,
R.F.; Schertler, G.F.; Weis, W.I.; Kobilka, B.K.
Deposited on : 2007-08-31
Resolution : 3.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

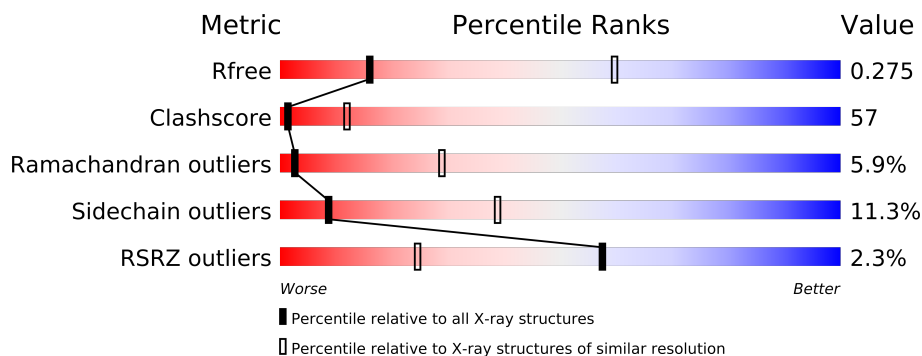
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
2	L	214	
3	H	217	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4925 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Beta-2 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1612	1052	271	279	10	0	0	0

- Molecule 2 is a protein called antibody for beta2 adrenoceptor, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1678	1050	278	341	9	0	0	0

- Molecule 3 is a protein called antibody for beta2 adrenoceptor, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	217	1635	1031	269	328	7	0	0	0

V211	P212	R213	D214	C215	G216	C217	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S160	V163	F166	P167	A168	V169	Q170	S171	D172	L174	T175	T176	L177	S178	S179	S180	V181	T182	V183	P184	S185	S186	T187	W188	P189	S190	E191	C195	M196	V197	A198	H199	P200	A201	S202	V206	T210	K67	V142	R143	G144	F145	F146	P147	E148	P149	T150	T151	V152	T153	F154	M155	S158	L159	S16
------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	338.38Å 48.48Å 89.35Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	19.99 – 3.40 85.92 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.99-3.40) 98.8 (85.92-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.270 0.226 , 0.275	Depositor DCC
R_{free} test set	1902 reflections (9.72%)	DCC
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 103.0	EDS
Estimated twinning fraction	0.039 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 19671 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4925	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.34	0/1636	0.57	0/2216
2	L	0.40	0/1716	0.73	0/2324
3	H	0.40	0/1677	0.74	1/2290 (0.0%)
All	All	0.38	0/5029	0.68	1/6830 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	141	LEU	CA-CB-CG	5.34	127.57	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1612	0	1610	195	0
2	L	1678	0	1610	208	0
3	H	1635	0	1578	177	0
All	All	4925	0	4798	556	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 57.

The worst 5 of 556 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:193:THR:HG23	2:L:208:SER:HB2	1.27	1.14
2:L:169:LYS:HD2	2:L:169:LYS:H	1.29	0.94
3:H:38:ARG:HB2	3:H:48:ILE:HD11	1.53	0.91
3:H:155:ASN:HB3	3:H:158:SER:HB2	1.53	0.90
2:L:38:GLN:HE21	3:H:39:GLN:HE22	1.16	0.89

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution. 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	204/365 (56%)	151 (74%)	39 (19%)	14 (7%)	2	24
2	L	212/214 (99%)	172 (81%)	31 (15%)	9 (4%)	4	41
3	H	215/217 (99%)	159 (74%)	42 (20%)	14 (6%)	2	25
All	All	631/796 (79%)	482 (76%)	112 (18%)	37 (6%)	2	29

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	LYS
1	A	142	GLN
1	A	143	SER
1	A	241	HIS
1	A	343	ARG

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 X-ray entries followed by that with respect to entries of similar resolution. 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	167/317 (53%)	151 (90%)	16 (10%)	12	49
2	L	191/191 (100%)	172 (90%)	19 (10%)	11	47
3	H	183/183 (100%)	157 (86%)	26 (14%)	5	27
All	All	541/691 (78%)	480 (89%)	61 (11%)	9	39

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	140	TYR
2	L	209	PHE
3	H	186	SER
2	L	144	ILE
2	L	157	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	52	ASN
2	L	137	ASN
3	H	6	GLN
2	L	38	GLN
2	L	198	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/365 (59%)	0.51	14 (6%) 18 7	26, 154, 221, 266	0
2	L	214/214 (100%)	-0.06	0 100 100	13, 58, 108, 171	0
3	H	217/217 (100%)	-0.01	1 (0%) 88 61	12, 57, 137, 198	0
All	All	647/796 (81%)	0.15	15 (2%) 57 24	12, 74, 197, 266	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	TRP	4.1
1	A	76	ALA	4.0
1	A	85	ALA	2.8
1	A	108	PHE	2.8
1	A	88	PRO	2.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.