



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:49 AM UTC

PDB ID : 3P2D / pdb\_00003p2d  
Title : Crystal structure of arrestin-3 reveals the basis of the difference in receptor binding between two non-visual subtypes  
Authors : Spiller, B.W.; Gurevich, V.V.; Zhan, X.; Gimenez, L.E.  
Deposited on : 2010-10-01  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

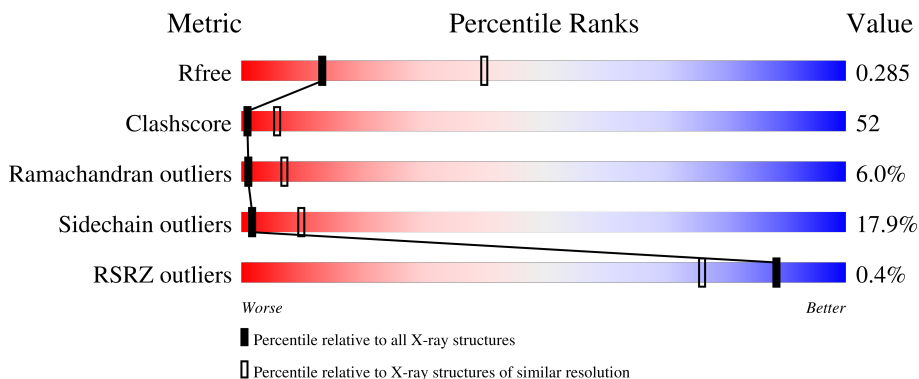
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	
1	B	393	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5611 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

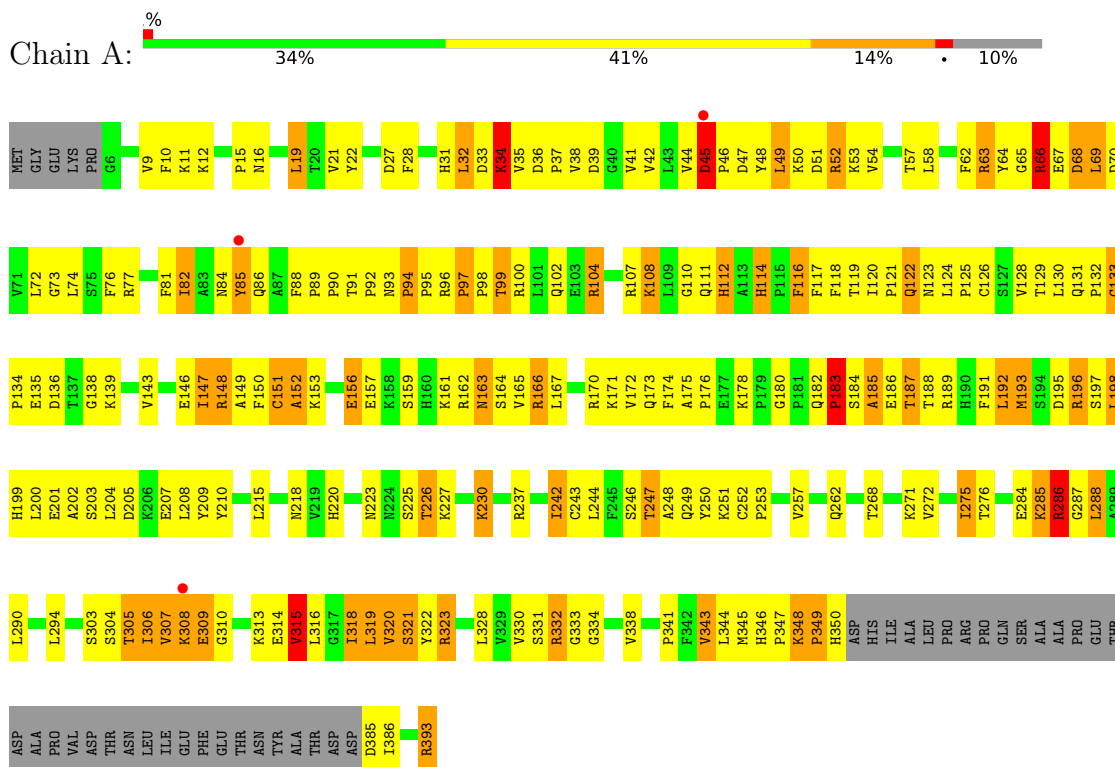
- Molecule 1 is a protein called Beta-arrestin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	Total 2814	C 1792	N 497	O 515	S 10	0	0	0
1	B	352	Total 2797	C 1781	N 493	O 513	S 10	0	0	0

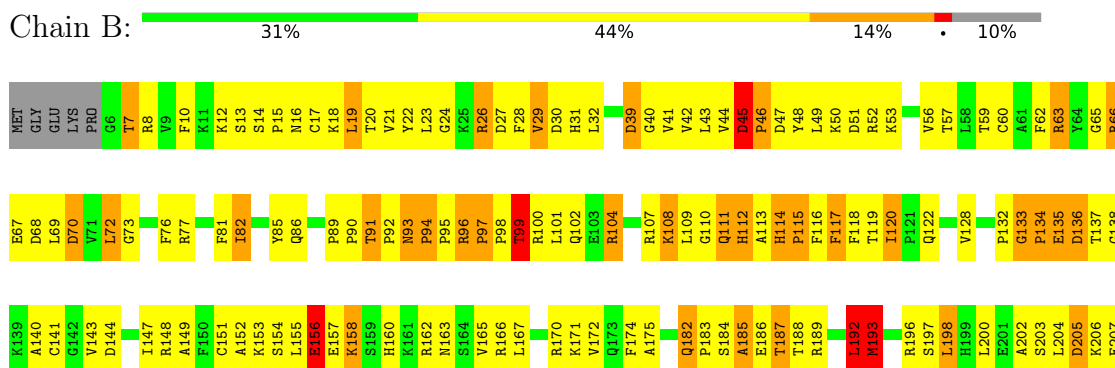
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Beta-arrestin-2



- Molecule 1: Beta-arrestin-2



L208	Y209	Y210	H211	G212	E213	P214	L215	N218	V219	H220	N223	N224	K227	T228	V229	K230	K231	I242	C243	L244	F245	S246	T247	A248	Q249	Y250	K251	Q256	V257	E258	Q259	D260	D261	Q262	V263	S264	P265	S266	S267	T268	F269	C270	K271	L278	L279	S280	N281	N282	R283	E284	K285	R286	G287	
L288	D291	L294	K295	H296	N300	T305	I306	V307	K308	E309	G310	A311	N312	K313	E314	V315	L316	G317	I318	L319	V320	R323	R324	V324	V325	L328	V329	V330	S331	R332	G333	G334	D335	V336	S337	V338	E339	L340	V343	L344	M345	H346	P347	K348	PRO	HIS	ASP	ASP	HIS	ILE	ALA	LEU	PRO	ARG
PRO	GLN	SER	ALA	ALA	PRO	GLU	THR	ASP	ALA	PRO	VAL	ASP	THR	ASN	LEU	ILE	GLU	PHE	GLU	THR	THR	ASN	TYR	ALA	THR	ASP	ASP	D385	I386	V387	F388	E389	D390	F391	A392	R393																		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.18Å 73.32Å 201.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.36 – 3.00 35.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (35.36-3.00) 92.6 (35.36-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.219 , 0.286 0.220 , 0.285	Depositor DCC
$R_{free}$ test set	1095 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.9	Xtrriage
Anisotropy	0.260	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 100.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5611	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	A	0.69	1/2878 (0.0%)	1.12	14/3897 (0.4%)
1	B	0.64	1/2859 (0.0%)	1.05	12/3870 (0.3%)
All	All	0.67	2/5737 (0.0%)	1.09	26/7767 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	ILE	CA-CB	-5.09	1.48	1.54
1	B	248	ALA	CA-CB	-5.01	1.45	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	ASN	N-CA-C	8.92	123.47	112.23
1	B	192	LEU	N-CA-C	-8.65	99.10	110.43
1	A	133	GLY	CA-C-N	8.39	130.33	119.84
1	A	133	GLY	C-N-CA	8.39	130.33	119.84
1	A	66	ARG	N-CA-C	-7.95	97.94	108.19

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	A	2814	0	2856	296	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2797	0	2842	298	0
All	All	5611	0	5698	590	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 52.

The worst 5 of 590 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)
1:B:41:VAL:HG22	1:B:115:PRO:HG3	1.19	1.15
1:A:53:LYS:HE2	1:A:86:GLN:HB3	1.13	1.12
1:A:49:LEU:HB2	1:A:52:ARG:HD2	1.32	1.11
1:B:40:GLY:O	1:B:115:PRO:HB3	1.53	1.07
1:A:348:LYS:HA	1:A:350:HIS:CD2	1.90	1.07

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 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	350/393 (89%)	282 (81%)	47 (13%)	21 (6%)	1	7
1	B	348/393 (88%)	293 (84%)	34 (10%)	21 (6%)	1	7
All	All	698/786 (89%)	575 (82%)	81 (12%)	42 (6%)	1	7

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	PRO
1	A	185	ALA
1	A	307	VAL

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Mol	Chain	Res	Type
1	A	308	LYS
1	A	348	LYS

### 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 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	320/353 (91%)	260 (81%)	60 (19%)	1	9
1	B	318/353 (90%)	264 (83%)	54 (17%)	2	11
All	All	638/706 (90%)	524 (82%)	114 (18%)	2	10

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	LEU
1	B	338	VAL
1	B	99	THR
1	B	332	ARG
1	B	283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	160	HIS
1	B	211	HIS
1	B	346	HIS
1	B	182	GLN
1	B	216	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

#### 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	354/393 (90%)	-0.36	3 (0%) 82 64	60, 99, 184, 286	0
1	B	352/393 (89%)	-0.34	0 100 100	66, 116, 206, 280	0
All	All	706/786 (89%)	-0.35	3 (0%) 88 76	60, 107, 198, 286	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	LYS	4.5
1	A	85	TYR	2.3
1	A	45	ASP	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.