



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 25, 2019 – 03:45 PM EST

PDB ID : 6PWC
EMDB ID: : EMD-20505
Title : A complex structure of arrestin-2 bound to neurotensin receptor 1
Authors : Yin, W.; Li, Z.; Jin, M.; Yin, Y.-L.; de Waal, P.W.; Pal, K.; Gao, X.; He, Y.;
Gao, J.; Wang, X.; Zhang, Y.; Zhou, H.; Melcher, K.; Jiang, Y.; Cong, Y.;
Zhou, X.E.; Yu, X.; Xu, H.E.
Deposited on : 2019-07-22
Resolution : 4.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

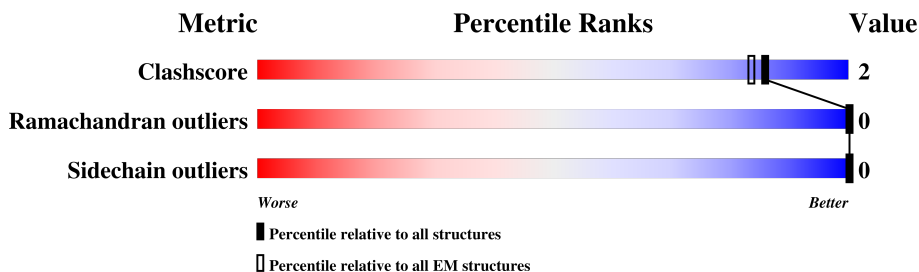
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	R	370	85% 13%
2	B	6	83% 17%
3	A	393	86% 11%
4	H	238	75% 7% 18%
5	L	215	81% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5879 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 Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	323	Total	C	N	O	S	0	0
			1824	1113	333	370	8		

- Molecule 2 is a protein called Neurotensin peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	5	Total	C	N	O	0	0
			27	17	5	5		

- Molecule 3 is a protein called Beta-arrestin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	350	Total	C	N	O	S	0	0
			1935	1188	350	388	9		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	CYS	VAL	conflict	UNP P49407
A	279	CYS	ALA	conflict	UNP P49407
A	386	ALA	ILE	conflict	UNP P49407
A	387	ALA	VAL	conflict	UNP P49407
A	388	ALA	PHE	conflict	UNP P49407

- Molecule 4 is a protein called Fab30 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	194	Total	C	N	O	S	0	0
			1072	639	194	234	5		

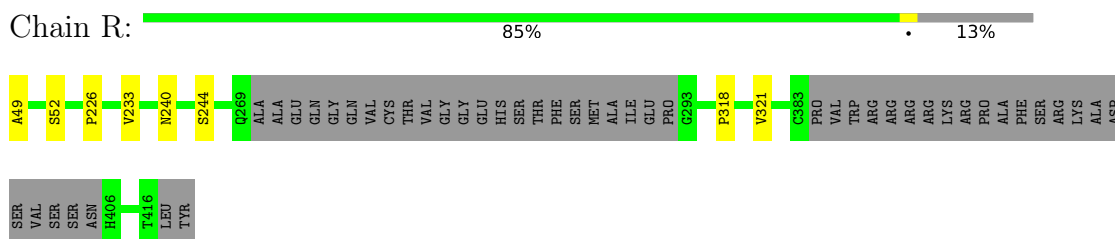
- Molecule 5 is a protein called Fab30 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	183	1021	605	183	230	3	0	0

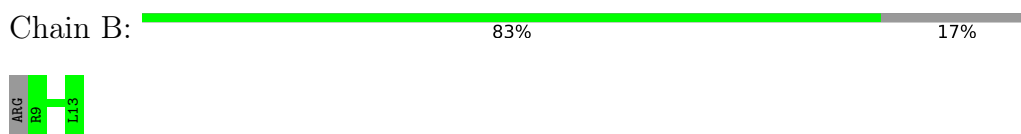
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

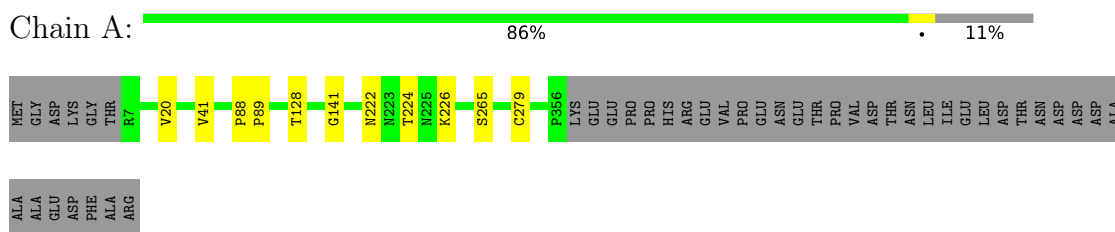
- Molecule 1: Neurotensin receptor type 1



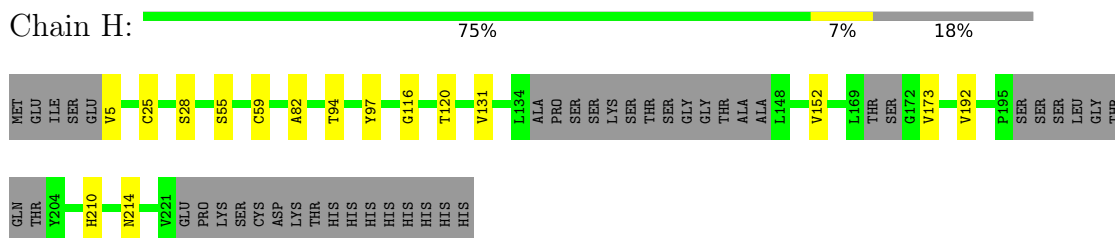
- Molecule 2: Neurotensin peptide



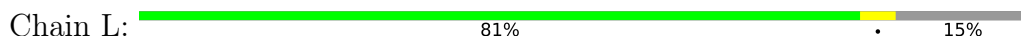
- Molecule 3: Beta-arrestin-1



- Molecule 4: Fab30 heavy chain



- Molecule 5: Fab30 light chain



S1	R19	V34	A52	I76	P121	K127	SER	GLY	THR	A131	S132	V133	V151	ASP	ASN	ALA	LEU	Q156	S160	T179	H190	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	260322	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 BASE (4k x 4k)	Depositor

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 >2	RMSZ	# Z >2
1	R	0.27	0/1840	0.44	0/2568
2	B	0.19	0/27	0.41	0/37
3	A	0.25	0/1963	0.49	0/2754
4	H	0.27	0/1077	0.52	0/1492
5	L	0.25	0/1028	0.49	0/1429
All	All	0.26	0/5935	0.48	0/8280

There are no bond length outliers.

There are no bond angle outliers.

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	R	1824	0	1303	4	0
2	B	27	0	14	0	0
3	A	1935	0	1324	7	0
4	H	1072	0	795	9	0
5	L	1021	0	741	4	0
All	All	5879	0	4177	23	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 2.

The worst 5 of 23 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)
5:L:19:ARG:HA	5:L:76:ILE:O	1.84	0.77
3:A:222:ASN:O	3:A:265:SER:HA	1.89	0.72
4:H:210:HIS:O	4:H:214:ASN:N	2.38	0.56
1:R:49:ALA:HB3	1:R:52:SER:HB3	1.87	0.56
1:R:318:PRO:HA	1:R:321:VAL:HB	1.89	0.55

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	R	317/370 (86%)	315 (99%)	2 (1%)	0	100	100
2	B	3/6 (50%)	3 (100%)	0	0	100	100
3	A	348/393 (88%)	342 (98%)	6 (2%)	0	100	100
4	H	186/238 (78%)	185 (100%)	1 (0%)	0	100	100
5	L	177/215 (82%)	173 (98%)	4 (2%)	0	100	100
All	All	1031/1222 (84%)	1018 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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 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	R	106/319 (33%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1/6 (17%)	1 (100%)	0	100	100
3	A	105/348 (30%)	105 (100%)	0	100	100
4	H	76/202 (38%)	76 (100%)	0	100	100
5	L	75/190 (40%)	75 (100%)	0	100	100
All	All	363/1065 (34%)	363 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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.