



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:14 PM GMT

PDB ID : 4BV0  
Title : High Resolution Structure of Evolved Agonist-bound Neurotensin Receptor 1  
Mutant without Lysozyme Fusion  
Authors : Egloff, P.; Hillenbrand, M.; Scott, D.J.; Schlinkmann, K.M.; Heine, P.; Balada,  
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Deposited on : 2013-06-24  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

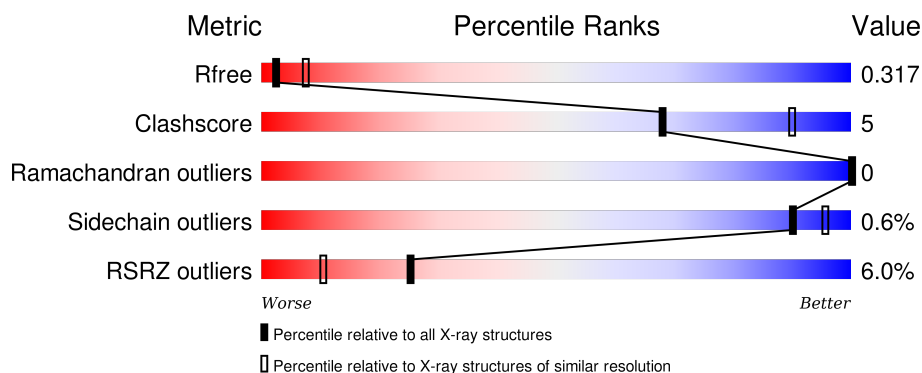
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	338	<div> <div>5%</div> <div>78% 9% 12%</div> </div>
1	B	338	<div> <div>6%</div> <div>78% 11% 11%</div> </div>
2	C	10	<div> <div>50% 20% 30%</div> </div>
2	D	10	<div> <div>40% 30% 30%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4865 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 NEUROTENSIN RECEPTOR TYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2348	1555	384	396	13			
1	B	302	Total	C	N	O	S	0	0	0
			2393	1585	391	403	14			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLY	-	EXPRESSION TAG	UNP P20789
A	47	PRO	-	EXPRESSION TAG	UNP P20789
A	48	GLY	-	EXPRESSION TAG	UNP P20789
A	49	SER	-	EXPRESSION TAG	UNP P20789
A	83	GLY	SER	ENGINEERED MUTATION	UNP P20789
A	86	LEU	ALA	ENGINEERED MUTATION	UNP P20789
A	101	ARG	THR	ENGINEERED MUTATION	UNP P20789
A	103	ASP	HIS	ENGINEERED MUTATION	UNP P20789
A	105	TYR	HIS	ENGINEERED MUTATION	UNP P20789
A	119	PHE	LEU	ENGINEERED MUTATION	UNP P20789
A	121	LEU	MET	ENGINEERED MUTATION	UNP P20789
A	124	ASP	GLU	ENGINEERED MUTATION	UNP P20789
A	125	VAL	LEU	ENGINEERED MUTATION	UNP P20789
A	143	LYS	ARG	ENGINEERED MUTATION	UNP P20789
A	150	GLU	ASP	ENGINEERED MUTATION	UNP P20789
A	161	VAL	ALA	ENGINEERED MUTATION	UNP P20789
A	167	LEU	ARG	ENGINEERED MUTATION	UNP P20789
A	172	ARG	CYS	ENGINEERED MUTATION	UNP P20789
A	177	HIS	ALA	ENGINEERED MUTATION	UNP P20789
A	208	VAL	MET	ENGINEERED MUTATION	UNP P20789
A	213	LEU	ARG	ENGINEERED MUTATION	UNP P20789
A	234	LEU	VAL	ENGINEERED MUTATION	UNP P20789
A	240	LEU	VAL	ENGINEERED MUTATION	UNP P20789
A	253	ALA	ILE	ENGINEERED MUTATION	UNP P20789
A	262	ARG	ASN	ENGINEERED MUTATION	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
A	263	ARG	LYS	ENGINEERED MUTATION	UNP P20789
A	.	-	VAL	DELETION	UNP P20789
A	.	-	GLY	DELETION	UNP P20789
A	.	-	THR	DELETION	UNP P20789
A	.	-	HIS	DELETION	UNP P20789
A	.	-	ASN	DELETION	UNP P20789
A	.	-	GLY	DELETION	UNP P20789
A	.	-	LEU	DELETION	UNP P20789
A	.	-	GLU	DELETION	UNP P20789
A	.	-	HIS	DELETION	UNP P20789
A	.	-	SER	DELETION	UNP P20789
A	.	-	THR	DELETION	UNP P20789
A	.	-	PHE	DELETION	UNP P20789
A	.	-	ASN	DELETION	UNP P20789
A	.	-	MET	DELETION	UNP P20789
A	.	-	THR	DELETION	UNP P20789
A	.	-	ILE	DELETION	UNP P20789
A	305	ARG	HIS	ENGINEERED MUTATION	UNP P20789
A	313	MET	VAL	ENGINEERED MUTATION	UNP P20789
A	332	VAL	CYS	ENGINEERED MUTATION	UNP P20789
A	342	ALA	PHE	ENGINEERED MUTATION	UNP P20789
A	354	SER	THR	ENGINEERED MUTATION	UNP P20789
A	358	VAL	PHE	ENGINEERED MUTATION	UNP P20789
A	362	ALA	SER	ENGINEERED MUTATION	UNP P20789
A	391	THR	-	EXPRESSION TAG	UNP P20789
A	392	ARG	-	EXPRESSION TAG	UNP P20789
A	393	GLU	-	EXPRESSION TAG	UNP P20789
A	394	LEU	-	EXPRESSION TAG	UNP P20789
A	395	GLU	-	EXPRESSION TAG	UNP P20789
A	396	VAL	-	EXPRESSION TAG	UNP P20789
A	397	LEU	-	EXPRESSION TAG	UNP P20789
A	398	PHE	-	EXPRESSION TAG	UNP P20789
A	399	GLN	-	EXPRESSION TAG	UNP P20789
B	46	GLY	-	EXPRESSION TAG	UNP P20789
B	47	PRO	-	EXPRESSION TAG	UNP P20789
B	48	GLY	-	EXPRESSION TAG	UNP P20789
B	49	SER	-	EXPRESSION TAG	UNP P20789
B	83	GLY	SER	ENGINEERED MUTATION	UNP P20789
B	86	LEU	ALA	ENGINEERED MUTATION	UNP P20789
B	101	ARG	THR	ENGINEERED MUTATION	UNP P20789
B	103	ASP	HIS	ENGINEERED MUTATION	UNP P20789
B	105	TYR	HIS	ENGINEERED MUTATION	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
B	119	PHE	LEU	ENGINEERED MUTATION	UNP P20789
B	121	LEU	MET	ENGINEERED MUTATION	UNP P20789
B	124	ASP	GLU	ENGINEERED MUTATION	UNP P20789
B	125	VAL	LEU	ENGINEERED MUTATION	UNP P20789
B	143	LYS	ARG	ENGINEERED MUTATION	UNP P20789
B	150	GLU	ASP	ENGINEERED MUTATION	UNP P20789
B	161	VAL	ALA	ENGINEERED MUTATION	UNP P20789
B	167	LEU	ARG	ENGINEERED MUTATION	UNP P20789
B	172	ARG	CYS	ENGINEERED MUTATION	UNP P20789
B	177	HIS	ALA	ENGINEERED MUTATION	UNP P20789
B	208	VAL	MET	ENGINEERED MUTATION	UNP P20789
B	213	LEU	ARG	ENGINEERED MUTATION	UNP P20789
B	234	LEU	VAL	ENGINEERED MUTATION	UNP P20789
B	240	LEU	VAL	ENGINEERED MUTATION	UNP P20789
B	253	ALA	ILE	ENGINEERED MUTATION	UNP P20789
B	262	ARG	ASN	ENGINEERED MUTATION	UNP P20789
B	263	ARG	LYS	ENGINEERED MUTATION	UNP P20789
B	.	-	VAL	DELETION	UNP P20789
B	.	-	GLY	DELETION	UNP P20789
B	.	-	THR	DELETION	UNP P20789
B	.	-	HIS	DELETION	UNP P20789
B	.	-	ASN	DELETION	UNP P20789
B	.	-	GLY	DELETION	UNP P20789
B	.	-	LEU	DELETION	UNP P20789
B	.	-	GLU	DELETION	UNP P20789
B	.	-	HIS	DELETION	UNP P20789
B	.	-	SER	DELETION	UNP P20789
B	.	-	THR	DELETION	UNP P20789
B	.	-	PHE	DELETION	UNP P20789
B	.	-	ASN	DELETION	UNP P20789
B	.	-	MET	DELETION	UNP P20789
B	.	-	THR	DELETION	UNP P20789
B	.	-	ILE	DELETION	UNP P20789
B	305	ARG	HIS	ENGINEERED MUTATION	UNP P20789
B	313	MET	VAL	ENGINEERED MUTATION	UNP P20789
B	332	VAL	CYS	ENGINEERED MUTATION	UNP P20789
B	342	ALA	PHE	ENGINEERED MUTATION	UNP P20789
B	354	SER	THR	ENGINEERED MUTATION	UNP P20789
B	358	VAL	PHE	ENGINEERED MUTATION	UNP P20789
B	362	ALA	SER	ENGINEERED MUTATION	UNP P20789
B	391	THR	-	EXPRESSION TAG	UNP P20789
B	392	ARG	-	EXPRESSION TAG	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
B	393	GLU	-	EXPRESSION TAG	UNP P20789
B	394	LEU	-	EXPRESSION TAG	UNP P20789
B	395	GLU	-	EXPRESSION TAG	UNP P20789
B	396	VAL	-	EXPRESSION TAG	UNP P20789
B	397	LEU	-	EXPRESSION TAG	UNP P20789
B	398	PHE	-	EXPRESSION TAG	UNP P20789
B	399	GLN	-	EXPRESSION TAG	UNP P20789

- Molecule 2 is a protein called NEUROTENSIN/NEUROMEDIN N.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			62	40	13	9			
2	D	7	Total	C	N	O	0	0	0
			62	40	13	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	GLY	-	EXPRESSION TAG	UNP P20068
C	5	PRO	-	EXPRESSION TAG	UNP P20068
C	6	GLY	-	EXPRESSION TAG	UNP P20068
C	7	GLY	-	EXPRESSION TAG	UNP P20068
D	4	GLY	-	EXPRESSION TAG	UNP P20068
D	5	PRO	-	EXPRESSION TAG	UNP P20068
D	6	GLY	-	EXPRESSION TAG	UNP P20068
D	7	GLY	-	EXPRESSION TAG	UNP P20068



GLY	PRO	GLY	RS	RG	L13



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.58 Å 91.56 Å 208.58 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 3.10 49.10 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.88-3.10) 95.3 (49.10-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 3.12 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.284 , 0.310 0.286 , 0.317	Depositor DCC
$R_{free}$ test set	1040 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	113.7	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 42.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 20790 reflections (0.019%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	0/2405	0.36	0/3281
1	B	0.23	0/2452	0.38	0/3345
2	C	0.17	0/63	0.38	0/82
2	D	0.17	0/63	0.38	0/82
All	All	0.22	0/4983	0.37	0/6790

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	A	2348	0	2416	19	0
1	B	2393	0	2462	27	0
2	C	62	0	66	1	0
2	D	62	0	66	3	0
All	All	4865	0	5010	46	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 5.

The worst 5 of 46 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:A:150:GLU:HG3	1:A:204:MET:HG3	1.73	0.70
1:B:54:ASP:O	2:D:8:ARG:NH2	2.30	0.64
1:A:208:VAL:HA	1:A:227:PRO:HA	1.84	0.60
1:B:239:GLN:OE1	1:B:333:TYR:OH	2.20	0.60
1:B:246:PHE:HD2	1:B:247:LEU:HD12	1.68	0.58

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	289/338 (86%)	278 (96%)	11 (4%)	0	100	100
1	B	294/338 (87%)	286 (97%)	8 (3%)	0	100	100
2	C	5/10 (50%)	5 (100%)	0	0	100	100
2	D	5/10 (50%)	5 (100%)	0	0	100	100
All	All	593/696 (85%)	574 (97%)	19 (3%)	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 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	256/290 (88%)	256 (100%)	0	100	100
1	B	262/290 (90%)	259 (99%)	3 (1%)	80	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	6/7 (86%)	6 (100%)	0	100	100
2	D	6/7 (86%)	6 (100%)	0	100	100
All	All	530/594 (89%)	527 (99%)	3 (1%)	90	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	ASP
1	B	86	LEU
1	B	142	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	325	HIS
1	B	219	HIS
1	B	325	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	297/338 (87%)	0.18	17 (5%) 27 11	24, 67, 153, 199	0
1	B	302/338 (89%)	0.25	20 (6%) 22 8	25, 77, 152, 256	0
2	C	7/10 (70%)	-0.18	0 100 100	53, 55, 105, 131	0
2	D	7/10 (70%)	0.53	0 100 100	58, 66, 100, 116	0
All	All	613/696 (88%)	0.21	37 (6%) 25 10	24, 73, 153, 256	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	THR	5.0
1	B	387	LEU	4.8
1	B	343	LEU	4.3
1	B	268	VAL	3.7
1	B	341	THR	3.4

### 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 carbohydrates 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.