



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:09 AM UTC

PDB ID : 2R1B / pdb_00002r1b
Title : Crystal Structure of rat neurexin 1beta with a splice insert at SS#4
Authors : Rudenko, G.
Deposited on : 2007-08-22
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

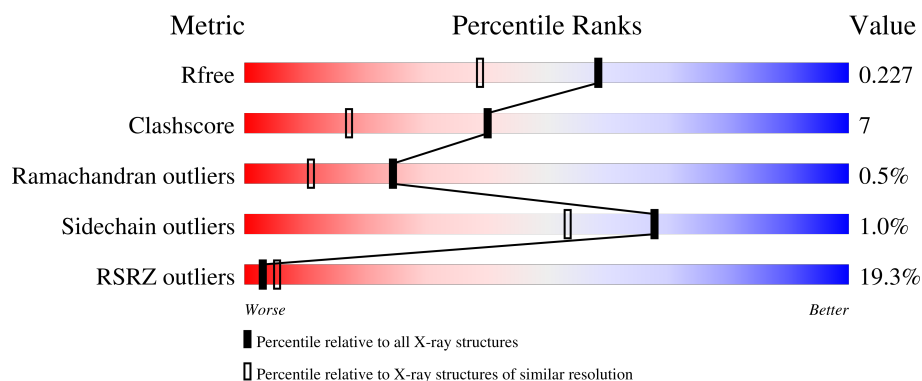
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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 ≥ 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	220	
1	B	220	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3378 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 Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	6	0
			1512	953	271	287	1			
1	B	196	Total	C	N	O	S	0	7	0
			1511	955	268	287	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLY	-	expression tag	UNP Q63373
A	76	SER	-	expression tag	UNP Q63373
B	75	GLY	-	expression tag	UNP Q63373
B	76	SER	-	expression tag	UNP Q63373

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

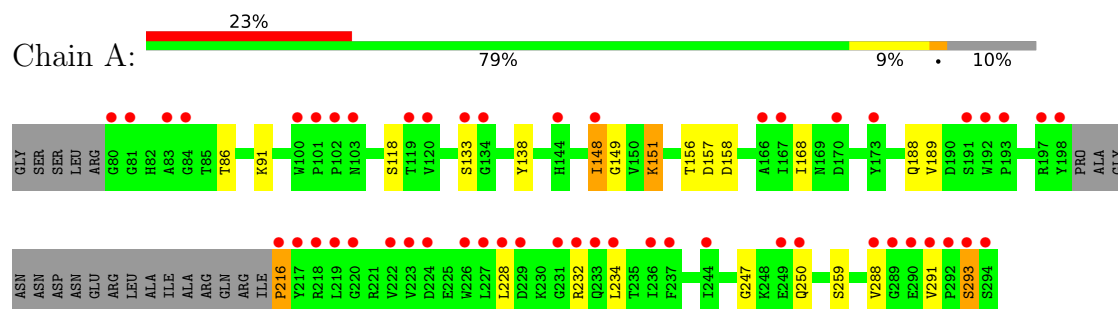
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total	O	0	0
			158	158		
3	B	195	Total	O	0	0
			195	195		

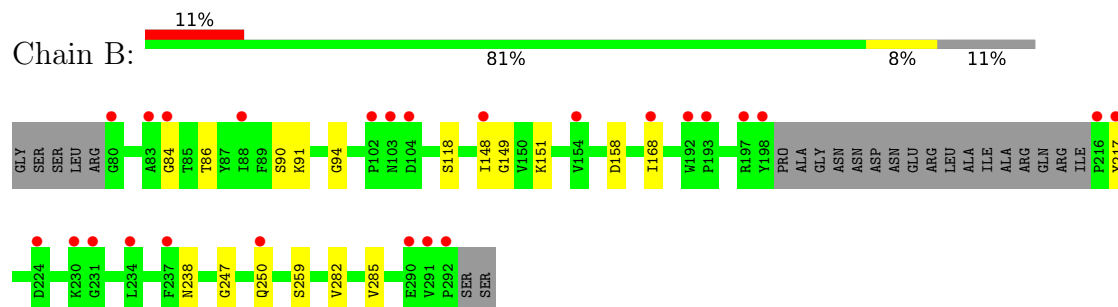
3 Residue-property plots [i](#)

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: Neurexin-1-beta



• Molecule 1: Neurexin-1-beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.12Å 39.26Å 85.41Å 90.00° 115.47° 90.00°	Depositor
Resolution (Å)	19.90 – 1.72 19.90 – 1.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.90-1.72) 91.8 (19.90-1.72)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.2, CNS	Depositor
R, R_{free}	0.197 , 0.225 0.202 , 0.227	Depositor DCC
R_{free} test set	3771 reflections (7.59%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3378	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.34	4/1562 (0.3%)	1.05	1/2115 (0.0%)
1	B	1.38	1/1565 (0.1%)	1.01	1/2118 (0.0%)
All	All	1.36	5/3127 (0.2%)	1.03	2/4233 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	PRO	N-CA	19.75	1.76	1.47
1	A	234	LEU	CG-CD1	5.38	1.70	1.52
1	A	188	GLN	N-CA	5.16	1.52	1.46
1	A	118	SER	N-CA	5.12	1.52	1.46
1	B	118	SER	N-CA	5.03	1.52	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	LYS	CB-CA-C	-6.79	108.73	116.54
1	B	238	ASN	N-CA-C	5.21	118.42	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	1512	0	1482	25	1
1	B	1511	0	1497	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	158	0	0	1	0
3	B	195	0	0	0	0
All	All	3378	0	2979	40	1

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 7.

All (40) 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:216:PRO:N	1:A:216:PRO:CA	1.76	1.45
1:B:247:GLY:HA2	1:B:250:GLN:NE2	1.49	1.26
1:B:247:GLY:HA2	1:B:250:GLN:HE22	1.00	1.06
1:A:247:GLY:HA2	1:A:250:GLN:NE2	1.69	1.06
1:B:148[B]:ILE:HG23	1:B:168:ILE:HG12	1.57	0.85
1:A:228:LEU:O	1:A:232[B]:ARG:HG3	1.79	0.83
1:A:247:GLY:HA2	1:A:250:GLN:HE22	1.45	0.80
1:A:228:LEU:HB3	1:A:232[B]:ARG:NH2	1.98	0.78
1:B:247:GLY:CA	1:B:250:GLN:NE2	2.43	0.77
1:B:247:GLY:CA	1:B:250:GLN:HE22	1.91	0.77
1:A:86[B]:THR:HG23	1:A:288:VAL:HB	1.66	0.76
1:A:247:GLY:HA2	1:A:250:GLN:HE21	1.49	0.73
1:A:148[B]:ILE:HG23	1:A:168:ILE:HG12	1.71	0.73
1:B:84:GLY:O	1:B:86[B]:THR:HG23	1.90	0.70
1:B:148[B]:ILE:HD12	1:B:149:GLY:N	2.14	0.63
1:A:291:VAL:C	1:A:293:SER:H	2.09	0.61
1:A:148[B]:ILE:HD12	1:A:149:GLY:N	2.19	0.57
1:A:247:GLY:CA	1:A:250:GLN:NE2	2.59	0.57
1:B:151[A]:LYS:HE2	1:B:158:ASP:HB3	1.87	0.56
1:A:156:THR:HG22	1:A:157:ASP:N	2.21	0.56
1:A:216:PRO:N	1:A:216:PRO:C	2.62	0.53
1:B:86[B]:THR:HG22	1:B:259:SER:HB3	1.91	0.53
1:B:86[A]:THR:HB	1:B:259:SER:HB3	1.93	0.51
1:A:86[A]:THR:HG23	1:A:259:SER:HB3	1.93	0.50
1:A:228:LEU:HD13	1:A:232[B]:ARG:NH2	2.27	0.49
1:A:291:VAL:C	1:A:293:SER:N	2.72	0.47
1:A:247:GLY:CA	1:A:250:GLN:HE22	2.23	0.45
1:A:138:TYR:OH	1:A:158:ASP:OD2	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HB3	1:A:232[B]:ARG:CZ	2.48	0.42
1:B:247:GLY:HA2	1:B:250:GLN:HE21	1.66	0.42
1:B:86[B]:THR:HG22	1:B:259:SER:CB	2.50	0.41
1:A:138:TYR:OH	1:A:151:LYS:HG2	2.21	0.41
1:A:228:LEU:HB3	1:A:232[B]:ARG:HH21	1.82	0.41
1:A:148[B]:ILE:HG12	1:A:189:VAL:HG22	2.03	0.41
1:A:232[A]:ARG:NH1	3:A:1060:HOH:O	2.28	0.41
1:B:90:SER:O	1:B:91:LYS:C	2.63	0.41
1:A:228:LEU:HD13	1:A:232[B]:ARG:HH22	1.85	0.41
1:B:94:GLY:HA3	1:B:285[A]:VAL:HG23	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:OG	1:A:232[B]:ARG:NH2[2_657]	2.15	0.05

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	200/220 (91%)	193 (96%)	6 (3%)	1 (0%)	24	11
1	B	199/220 (90%)	194 (98%)	4 (2%)	1 (0%)	24	11
All	All	399/440 (91%)	387 (97%)	10 (2%)	2 (0%)	24	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	SER
1	B	217	TYR

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	159/178 (89%)	156 (98%)	3 (2%)	50	27
1	B	162/178 (91%)	160 (99%)	2 (1%)	63	46
All	All	321/356 (90%)	316 (98%)	5 (2%)	68	34

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148[A]	ILE
1	A	148[B]	ILE
1	A	151	LYS
1	B	282[A]	VAL
1	B	282[B]	VAL

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

Mol	Chain	Res	Type
1	A	144	HIS
1	A	250	GLN
1	B	184	ASN
1	B	250	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	198/220 (90%)	1.54	51 (25%) 1 3	15, 25, 35, 43	6 (3%)
1	B	196/220 (89%)	1.09	25 (12%) 7 11	16, 25, 35, 43	7 (3%)
All	All	394/440 (89%)	1.31	76 (19%) 3 5	15, 25, 35, 43	13 (3%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	PRO	6.9
1	B	216	PRO	6.5
1	B	80	GLY	5.1
1	A	231	GLY	4.9
1	A	198	TYR	4.6
1	A	217	TYR	4.6
1	A	80	GLY	4.2
1	A	294	SER	4.2
1	A	102	PRO	4.1
1	A	226	TRP	4.0
1	A	293	SER	3.9
1	A	237	PHE	3.9
1	A	84	GLY	3.8
1	A	218	ARG	3.8
1	A	83	ALA	3.8
1	A	219	LEU	3.7
1	A	103	ASN	3.6
1	A	133	SER	3.6
1	A	234	LEU	3.5
1	A	192	TRP	3.5
1	A	222	VAL	3.4
1	B	292	PRO	3.4
1	A	223	VAL	3.4
1	A	292	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	101	PRO	3.3
1	B	84	GLY	3.3
1	A	291	VAL	3.3
1	B	217	TYR	3.3
1	B	103	ASN	3.3
1	A	228	LEU	3.2
1	A	220	GLY	3.2
1	B	198	TYR	3.2
1	A	229	ASP	3.0
1	A	167	ILE	3.0
1	A	290	GLU	2.9
1	A	227	LEU	2.9
1	A	120	VAL	2.8
1	A	250	GLN	2.7
1	B	250	GLN	2.7
1	A	166	ALA	2.7
1	A	81	GLY	2.6
1	B	197	ARG	2.6
1	A	232[A]	ARG	2.6
1	A	197	ARG	2.6
1	A	288	VAL	2.5
1	B	290	GLU	2.5
1	B	291	VAL	2.5
1	A	191	SER	2.5
1	A	173	TYR	2.5
1	A	144	HIS	2.5
1	A	236	ILE	2.4
1	B	83	ALA	2.4
1	B	104	ASP	2.4
1	B	231	GLY	2.4
1	A	100	TRP	2.4
1	A	148[A]	ILE	2.4
1	A	244	ILE	2.4
1	A	233	GLN	2.3
1	A	134	GLY	2.3
1	B	230	LYS	2.3
1	B	237	PHE	2.3
1	A	249	GLU	2.3
1	B	234	LEU	2.3
1	B	154	VAL	2.3
1	B	88	ILE	2.2
1	B	192	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	119	THR	2.1
1	A	170	ASP	2.1
1	A	224	ASP	2.1
1	B	224	ASP	2.1
1	A	193	PRO	2.1
1	B	102	PRO	2.1
1	B	168	ILE	2.1
1	A	289	GLY	2.1
1	B	193	PRO	2.1
1	B	148[A]	ILE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	1001	1/1	0.96	0.16	24,24,24,24	0
2	CA	B	1002	1/1	0.99	0.21	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.