Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 01:04 PM EDT

PDB ID	:	2R1B
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 (i) 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 (1)) were used in the production of this report:

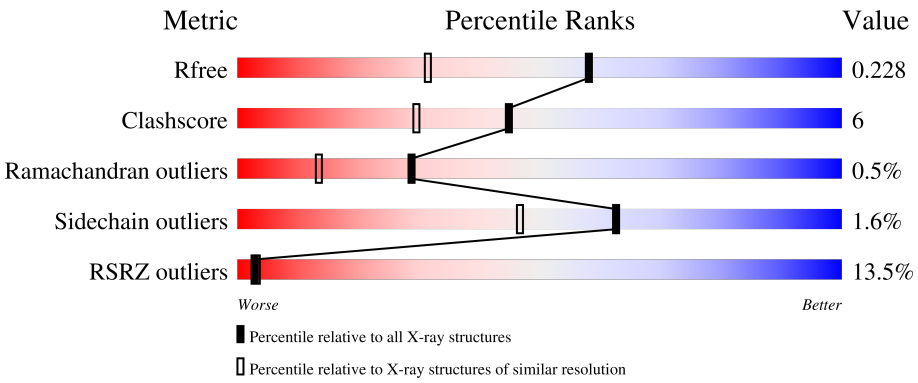
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 <=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	15%; 80%; 8% • 10%
1	B	220	10%; 80%; 8% • 11%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	198	1512	953	271	287	1	0	6	0
1	B	196	1511	955	268	287	1	0	7	0

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

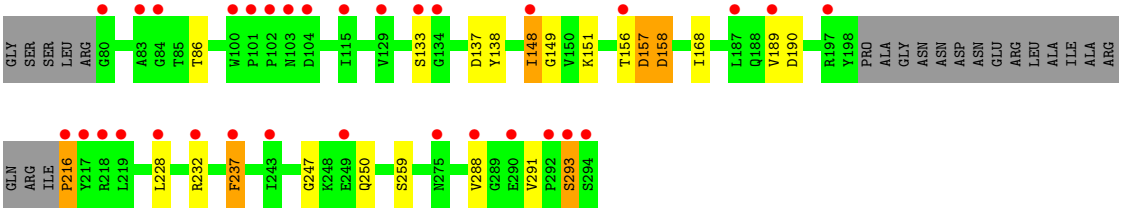
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	158	158	158	0	0
3	B	195	195	195	0	0

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.

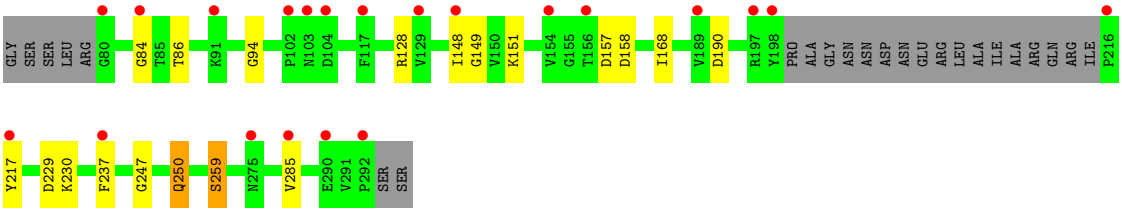
• Molecule 1: Neurexin-1-beta

Chain A:



• Molecule 1: Neurexin-1-beta

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.92 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.2, CNS	Depositor
R, R_{free}	0.197 , 0.225 0.202 , 0.228	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)	0.36 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	1.11	2/1562 (0.1%)	0.92	4/2115 (0.2%)
1	B	1.10	1/1565 (0.1%)	0.92	4/2118 (0.2%)
All	All	1.10	3/3127 (0.1%)	0.92	8/4233 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	PRO	N-CA	17.31	1.76	1.47
1	A	237	PHE	CE2-CZ	6.42	1.49	1.37
1	B	259	SER	CB-OG	5.81	1.49	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	157	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	137	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	128	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	B	190	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	157	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	158	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	229	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	190	ASP	CB-CG-OD2	5.11	122.90	118.30

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	1512	0	1482	25	1
1	B	1511	0	1497	14	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	39	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 6.

All (39) 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: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:291:VAL:C	1:A:293:SER:H	2.09	0.56
1:A:156:THR:HG22	1:A:157:ASP:N	2.21	0.56
1:B:86[B]:THR:HG22	1:B:259:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:PRO:N	1:A:216:PRO:C	2.62	0.49
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
1:A:291:VAL:C	1:A:293:SER:N	2.72	0.43
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: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 (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	200/220 (91%)	193 (96%)	6 (3%)	1 (0%)	29 13
1	B	199/220 (90%)	194 (98%)	4 (2%)	1 (0%)	29 13
All	All	399/440 (91%)	387 (97%)	10 (2%)	2 (0%)	29 13

All (2) Ramachandran outliers are listed below:

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

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	159/178 (89%)	156 (98%)	3 (2%)	57	39
1	B	162/178 (91%)	159 (98%)	3 (2%)	57	39
All	All	321/356 (90%)	315 (98%)	6 (2%)	62	39

All (6) 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	237	PHE
1	B	230	LYS
1	B	237	PHE
1	B	250	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	250	GLN
1	B	184	ASN
1	B	240	GLN
1	B	250	GLN
1	B	257	GLN

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 monosaccharides 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 (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, 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%)	1.05	32 (16%)	1	1	17, 25, 35, 43	0
1	B	196/220 (89%)	0.87	21 (10%)	6	6	18, 25, 35, 43	0
All	All	394/440 (89%)	0.96	53 (13%)	3	3	17, 25, 35, 43	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	PRO	6.3
1	A	293	SER	6.2
1	A	103	ASN	6.0
1	B	80	GLY	5.8
1	A	237	PHE	5.8
1	B	216	PRO	5.4
1	A	294	SER	5.3
1	A	217	TYR	5.0
1	B	103	ASN	4.6
1	B	148[A]	ILE	4.5
1	A	102	PRO	4.5
1	A	84	GLY	4.5
1	A	80	GLY	4.3
1	A	133	SER	4.1
1	A	148[A]	ILE	3.6
1	A	104	ASP	3.5
1	A	292	PRO	3.4
1	B	217	TYR	3.4
1	A	218	ARG	3.3
1	B	84	GLY	3.3
1	B	104	ASP	3.2
1	A	101	PRO	2.9
1	B	237	PHE	2.8
1	A	129	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	83	ALA	2.7
1	A	275	ASN	2.7
1	B	91	LYS	2.7
1	B	154	VAL	2.5
1	A	290	GLU	2.5
1	B	156	THR	2.5
1	B	197	ARG	2.5
1	A	232[A]	ARG	2.4
1	A	249	GLU	2.4
1	B	102	PRO	2.4
1	A	288	VAL	2.4
1	A	228	LEU	2.4
1	A	187	LEU	2.2
1	A	219	LEU	2.2
1	B	198	TYR	2.2
1	A	156	THR	2.2
1	B	129	VAL	2.2
1	B	117	PHE	2.2
1	A	189	VAL	2.2
1	B	275	ASN	2.2
1	A	197	ARG	2.1
1	B	285[A]	VAL	2.1
1	B	290	GLU	2.1
1	A	243	ILE	2.1
1	B	292	PRO	2.0
1	A	115	ILE	2.0
1	A	134	GLY	2.0
1	B	189	VAL	2.0
1	A	100	TRP	2.0

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 monosaccharides 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(Å^2)	Q<0.9
2	CA	A	1001	1/1	0.98	0.13	24,24,24,24	0
2	CA	B	1002	1/1	0.99	0.15	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.