wwPDB X-ray Structure Validation Summary Report (i)

May 24, 2020 – 05:59 pm BST

PDB ID	:	1C4R
Title	:	THE STRUCTURE OF THE LIGAND-BINDING DOMAIN OF NEUREXIN 1BETA: REGULATION OF LNS DOMAIN FUNCTION BY ALTERNATIVE SPLICING
Authors	:	Rudenko, G.; Nguyen, T.; Chelliah, Y.; Sudhof, T.C.; Deisenhofer, J.
Deposited on	:	1999-09-28
Resolution	:	2.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

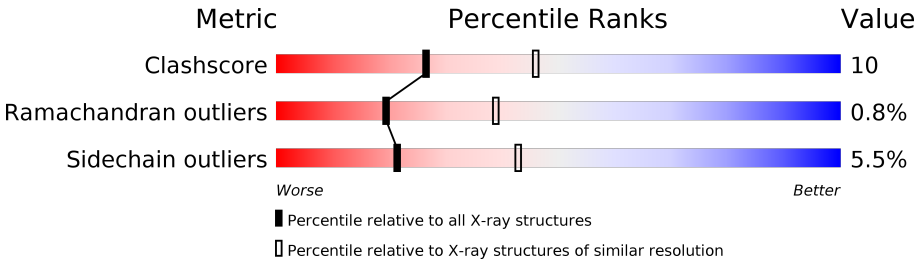
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 >=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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	182	73% 23%
1	B	182	79% 17%
1	C	182	79% 17%
1	D	182	78% 16%
1	E	182	75% 23%
1	F	182	76% 17%
1	G	182	78% 20%
1	H	182	76% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11086 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-I BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	14	0	0
			1379	869	246	263	1			
1	B	178	Total	C	N	O	S	15	0	0
			1363	859	244	259	1			
1	C	180	Total	C	N	O	S	19	0	0
			1379	869	246	263	1			
1	D	178	Total	C	N	O	S	15	0	0
			1363	859	244	259	1			
1	E	181	Total	C	N	O	S	21	0	0
			1386	874	247	264	1			
1	F	177	Total	C	N	O	S	20	0	0
			1359	857	243	258	1			
1	G	182	Total	C	N	O	S	10	0	0
			1390	876	248	265	1			
1	H	177	Total	C	N	O	S	14	0	0
			1359	857	243	258	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	19	Total	O	0	0
			19	19		
2	C	11	Total	O	0	0
			11	11		
2	D	21	Total	O	0	0
			21	21		
2	E	8	Total	O	0	0
			8	8		
2	F	14	Total	O	0	0
			14	14		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	13	Total O 13 13	0	0
2	H	14	Total O 14 14	0	0

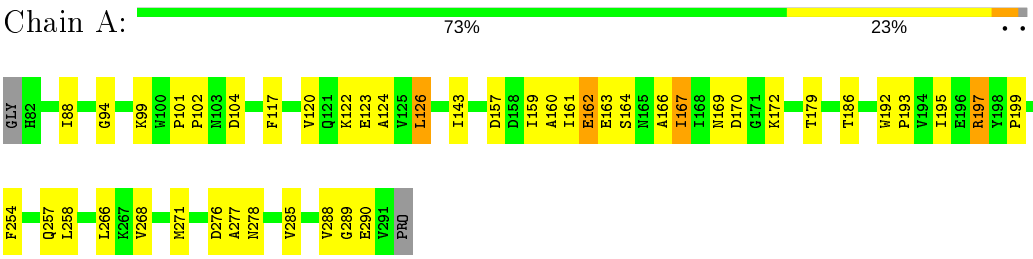
3 Residue-property plots (i)

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.

Note EDS was not executed.

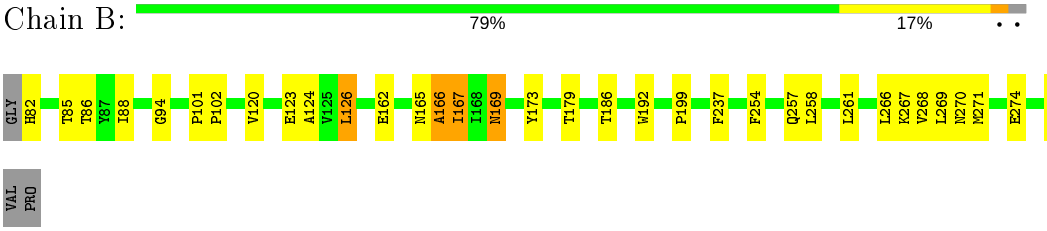
- Molecule 1: NEUREXIN-I BETA

Chain A:



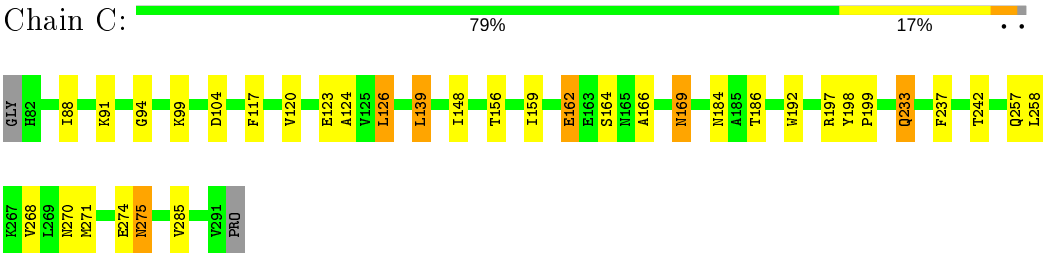
- Molecule 1: NEUREXIN-I BETA

Chain B:



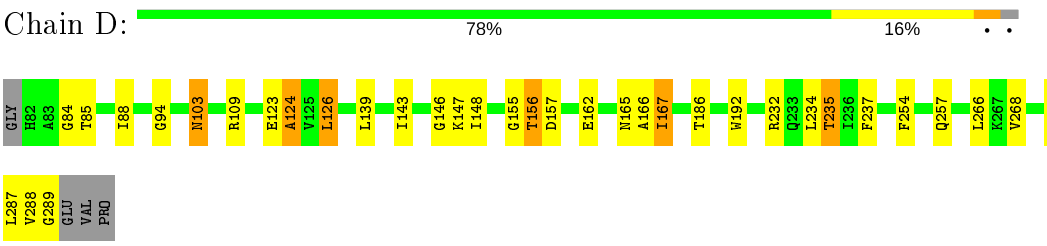
- Molecule 1: NEUREXIN-I BETA

Chain C:



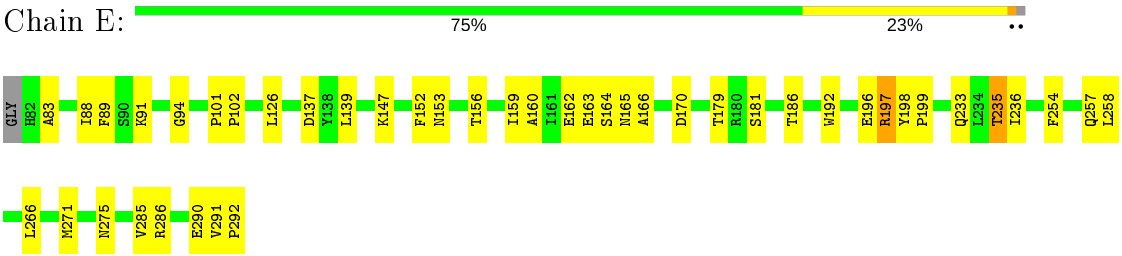
- Molecule 1: NEUREXIN-I BETA

Chain D:



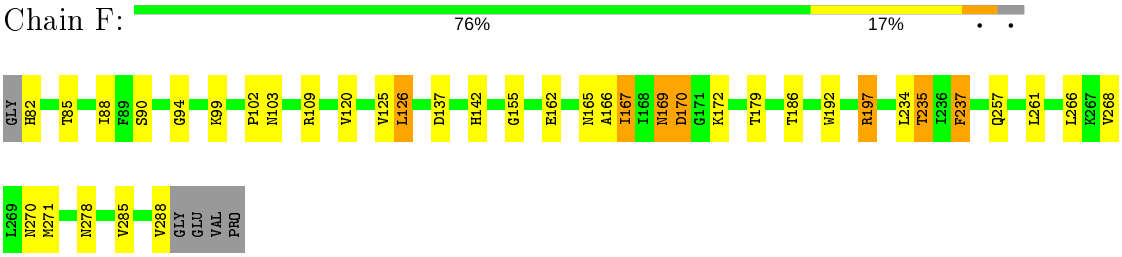
• Molecule 1: NEUREXIN-I BETA

Chain E:



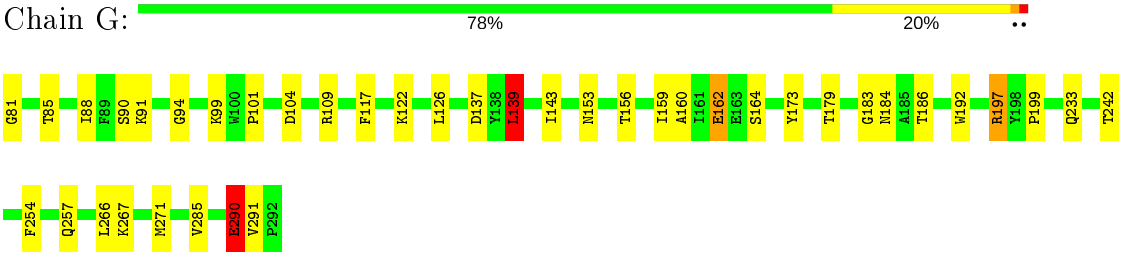
• Molecule 1: NEUREXIN-I BETA

Chain F:



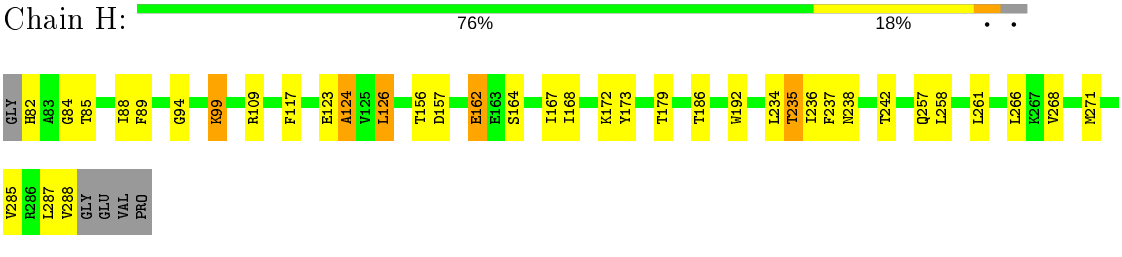
• Molecule 1: NEUREXIN-I BETA

Chain G:



• Molecule 1: NEUREXIN-I BETA

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.60Å 195.90Å 103.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.9 (20.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11086	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.64	0/1405	0.81	2/1904 (0.1%)
1	B	0.72	0/1389	0.88	1/1882 (0.1%)
1	C	0.63	0/1405	0.85	1/1904 (0.1%)
1	D	0.69	0/1389	0.88	1/1882 (0.1%)
1	E	0.67	1/1413 (0.1%)	0.83	0/1916
1	F	0.66	0/1385	0.92	2/1877 (0.1%)
1	G	0.74	1/1417 (0.1%)	0.88	1/1921 (0.1%)
1	H	0.67	0/1385	0.89	2/1877 (0.1%)
All	All	0.68	2/11188 (0.0%)	0.87	10/15163 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	290	GLU	CD-OE1	5.66	1.31	1.25
1	G	290	GLU	CB-CG	5.29	1.62	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	139	LEU	CA-CB-CG	7.72	133.06	115.30
1	H	126	LEU	CA-CB-CG	7.11	131.66	115.30
1	D	232	ARG	N-CA-C	-7.01	92.06	111.00
1	G	139	LEU	CA-CB-CG	6.03	129.18	115.30
1	H	238	ASN	N-CA-C	5.90	126.94	111.00

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	1379	0	1365	32	0
1	B	1363	0	1350	26	0
1	C	1379	0	1365	24	0
1	D	1363	0	1350	31	0
1	E	1386	0	1372	31	0
1	F	1359	0	1347	29	0
1	G	1390	0	1375	27	0
1	H	1359	0	1347	26	0
2	A	8	0	0	0	0
2	B	19	0	0	0	0
2	C	11	0	0	1	0
2	D	21	0	0	1	0
2	E	8	0	0	0	0
2	F	14	0	0	0	0
2	G	13	0	0	0	0
2	H	14	0	0	0	0
All	All	11086	0	10871	221	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 10.

The worst 5 of 221 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:C:156:THR:HB	1:C:233:GLN:HG3	1.38	1.04
1:H:109:ARG:HG2	1:H:235:THR:HG23	1.49	0.94
1:A:192:TRP:HB3	1:A:193:PRO:HD2	1.49	0.92
1:D:166:ALA:HB3	1:D:192:TRP:CZ3	2.06	0.90
1:B:120:VAL:C	1:B:169:ASN:HD21	1.79	0.85

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	178/182 (98%)	165 (93%)	13 (7%)	0	100	100
1	B	176/182 (97%)	164 (93%)	11 (6%)	1 (1%)	25	47
1	C	178/182 (98%)	168 (94%)	9 (5%)	1 (1%)	25	47
1	D	176/182 (97%)	162 (92%)	12 (7%)	2 (1%)	14	30
1	E	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	14	30
1	F	175/182 (96%)	162 (93%)	10 (6%)	3 (2%)	9	18
1	G	180/182 (99%)	168 (93%)	11 (6%)	1 (1%)	25	47
1	H	175/182 (96%)	161 (92%)	13 (7%)	1 (1%)	25	47
All	All	1417/1456 (97%)	1318 (93%)	88 (6%)	11 (1%)	19	39

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	156	THR
1	G	85	THR
1	B	166	ALA
1	E	83	ALA
1	F	102	PRO

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	145/146 (99%)	138 (95%)	7 (5%)	25	49
1	B	143/146 (98%)	136 (95%)	7 (5%)	25	48
1	C	145/146 (99%)	135 (93%)	10 (7%)	15	31
1	D	143/146 (98%)	135 (94%)	8 (6%)	21	42
1	E	146/146 (100%)	138 (94%)	8 (6%)	21	43
1	F	143/146 (98%)	133 (93%)	10 (7%)	15	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	146/146 (100%)	139 (95%)	7 (5%)	25 49
1	H	143/146 (98%)	136 (95%)	7 (5%)	25 48
All	All	1154/1168 (99%)	1090 (94%)	64 (6%)	21 43

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	167	ILE
1	E	186	THR
1	H	162	GLU
1	D	186	THR
1	E	162	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	103	ASN
1	D	238	ASN
1	F	103	ASN
1	C	275	ASN
1	F	270	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.