



Full wwPDB NMR Structure Validation Report ⓘ

Feb 18, 2018 – 08:43 am GMT

PDB ID : 1XR0
Title : Structural Basis of SNT PTB Domain Interactions with Distinct Neurotrophic Receptors
Authors : Dhalluin, C.; Yan, K.S.; Plotnikova, O.; Lee, K.W.; Zeng, L.; Kuti, M.; Mujtaba, S.; Goldfarb, M.P.; Zhou, M.-M.
Deposited on : 2004-10-13

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

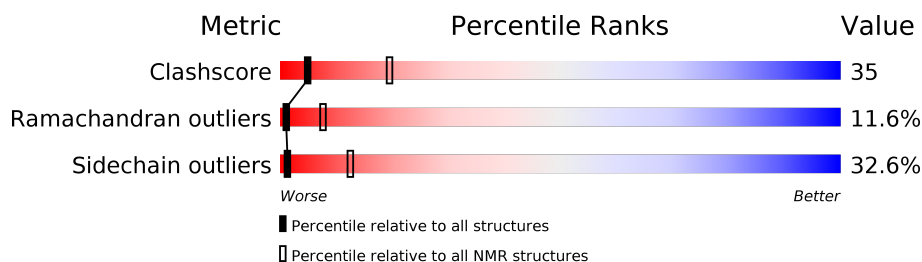
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	A	22	 41% 41% 18%
2	B	129	 34% 49% 16% .

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2436 atoms, of which 1211 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Basic fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	22	Total	C	H	N	O	S	0
			368	108	194	36	29	1	

- Molecule 2 is a protein called FGFR signalling adaptor SNT-1.

Mol	Chain	Residues	Atoms						Trace
2	B	129	Total	C	H	N	O	S	0
			2068	649	1017	190	205	7	

There are 3 discrepancies between the modelled and reference sequences:

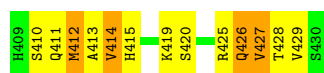
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	CLONING ARTIFACT	UNP Q8WU20
B	9	GLY	-	CLONING ARTIFACT	UNP Q8WU20
B	10	SER	-	CLONING ARTIFACT	UNP Q8WU20

4 Residue-property plots

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

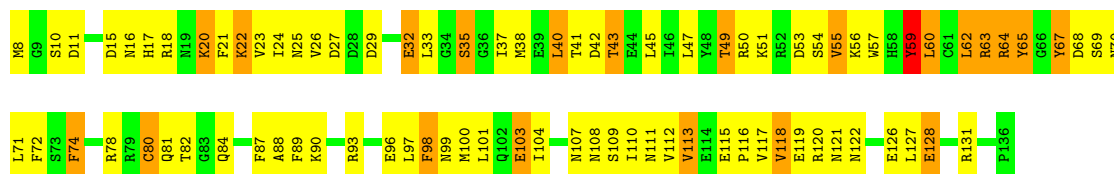
- Molecule 1: Basic fibroblast growth factor receptor 1

Chain A: 



- Molecule 2: FGFR signalling adaptor SNT-1

Chain B: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Structures of the SNT-1 PTB domain in complex with the hFGFR1 peptide were calculated with a distance geometry and simulated annealing protocol by using the X-PLOR program ([4]). NOE distance and dihedral angle restraints were treated with a square-well potential of 50 kcal mol⁻¹. A total of 2448 manually assigned NOE-derived distance restraints were obtained from the 15N- or 13C-edited NOESY data. Included in this figure are 251 intrapeptide and 258 intermolecular distance restraints. Additionally, 255 unambiguous and 52 ambiguous distance restraints were identified from the NOE data by using ARIA. The final structure calculations employed a total of 2755 NOE restraints obtained from the manual and the ARIA-assisted assignments, 2703 of which were unambiguously assigned NOE-derived distance restraints that comprise 1072 intraresidue, 466 sequential, 216 medium-range, and 949 long-range NOEs. In addition, 70 hydrogen-bond distance restraints for 35 hydrogen bonds and 19 γ -angle restraints were also used in the structure calculations. For the ensemble of the final 20 structures, no distance or torsional angle restraint was violated by more than 0.4 or 5, respectively. The distance-violation, dihedral-violation, and total energies were 74.4 1.7 kcal mol⁻¹, 0.82 0.08 kcal mol⁻¹, and 262.0 6.0 kcal mol⁻¹, respectively. The Lennard-Jones potential, which was not used during any refinement stage, was 659.3 23.1 kcal mol⁻¹ for the final structures. Ramachandran plot analysis by Procheck-NMR showed that in the final structures of the complex, 98.1% of the backbone geometries of the non-Gly and non-Pro residues in the complex (protein residues 18-116 and peptide residues 412-430) and nearly 100% in the secondary structure (protein residues 19-24, 35-40, 45-49, 52-57, 63-68, 71-76, 85-90, 94-107, and 111-115 and peptide residues 426-430) lie within energetically favorable or allowed regions..*

Of the 100 calculated structures, 1 were deposited, based on the following criterion: *structures with the least restraint violations.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	structure solution	3.851
ARIA	refinement	1.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	174	194	189	27
2	B	1051	1017	1011	82
All	All	1225	1211	1200	86

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 35.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:414:VAL:HG13	2:B:82:THR:HG21	0.98	1.35
2:B:47:LEU:HD21	2:B:89:PHE:CZ	0.82	2.09
1:A:414:VAL:CG1	2:B:82:THR:HG21	0.76	2.11
1:A:428:THR:O	2:B:113:VAL:HG22	0.75	1.81
1:A:428:THR:HG23	2:B:64:ARG:HG2	0.70	1.63
2:B:26:VAL:HG11	2:B:90:LYS:CD	0.69	2.17
2:B:26:VAL:HG11	2:B:90:LYS:HD2	0.69	1.63
2:B:26:VAL:HG22	2:B:88:ALA:O	0.69	1.88
1:A:413:ALA:HB2	2:B:49:THR:CB	0.67	2.18
2:B:45:LEU:HD13	2:B:59:TYR:CD1	0.63	2.29
2:B:27:ASP:HB3	2:B:33:LEU:HD21	0.63	1.71
2:B:40:LEU:HD21	2:B:97:LEU:HG	0.61	1.70
2:B:60:LEU:HB3	2:B:110:ILE:HD13	0.61	1.72
1:A:428:THR:HB	2:B:113:VAL:HG23	0.60	1.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:26:VAL:HG23	2:B:88:ALA:HB3	0.59	1.75
2:B:65:TYR:CE2	2:B:98:PHE:CD1	0.58	2.91
2:B:65:TYR:CE2	2:B:101:LEU:HD23	0.57	2.35
1:A:414:VAL:CG1	2:B:55:VAL:HG11	0.56	2.30
1:A:414:VAL:HG13	2:B:82:THR:CG2	0.55	2.24
1:A:413:ALA:HB2	2:B:49:THR:OG1	0.55	2.01
1:A:414:VAL:CG2	2:B:87:PHE:CG	0.54	2.91
2:B:40:LEU:HD23	2:B:101:LEU:HD13	0.54	1.79
1:A:429:VAL:HB	2:B:112:VAL:HG12	0.53	1.80
2:B:42:ASP:O	2:B:43:THR:HG23	0.52	2.04
2:B:45:LEU:CD1	2:B:59:TYR:CE1	0.52	2.92
2:B:65:TYR:CZ	2:B:98:PHE:CE1	0.52	2.98
2:B:25:ASN:O	2:B:33:LEU:HD12	0.52	2.04
2:B:65:TYR:CE2	2:B:101:LEU:CD2	0.51	2.93
1:A:413:ALA:HB2	2:B:49:THR:HB	0.51	1.81
1:A:414:VAL:HG13	1:A:414:VAL:O	0.51	2.06
2:B:71:LEU:HD23	2:B:71:LEU:C	0.51	2.25
2:B:97:LEU:HD23	2:B:98:PHE:N	0.51	2.21
2:B:65:TYR:CE2	2:B:98:PHE:CE1	0.50	3.00
2:B:97:LEU:C	2:B:97:LEU:HD23	0.50	2.26
2:B:45:LEU:CD1	2:B:59:TYR:CD1	0.50	2.95
1:A:429:VAL:CG1	2:B:65:TYR:CD1	0.49	2.96
2:B:55:VAL:O	2:B:57:TRP:CZ3	0.49	2.66
1:A:414:VAL:HG12	2:B:55:VAL:HG11	0.48	1.84
2:B:110:ILE:HG22	2:B:111:ASN:N	0.48	2.22
2:B:65:TYR:CD1	2:B:65:TYR:O	0.48	2.67
2:B:65:TYR:CD2	2:B:101:LEU:HD23	0.48	2.44
1:A:428:THR:HG23	2:B:64:ARG:CG	0.48	2.36
2:B:20:LYS:O	2:B:21:PHE:CD1	0.47	2.67
2:B:49:THR:HG23	2:B:53:ASP:O	0.47	2.08
2:B:113:VAL:HG23	2:B:113:VAL:O	0.47	2.10
2:B:24:ILE:O	2:B:89:PHE:CD1	0.47	2.68
2:B:22:LYS:HA	2:B:37:ILE:HD13	0.47	1.86
1:A:414:VAL:HG23	2:B:87:PHE:HB3	0.46	1.86
2:B:74:PHE:CD1	2:B:87:PHE:HB2	0.46	2.45
1:A:415:HIS:HB2	2:B:33:LEU:HD11	0.46	1.87
1:A:429:VAL:CG2	1:A:429:VAL:O	0.46	2.63
1:A:414:VAL:CG1	2:B:82:THR:CG2	0.45	2.92
2:B:26:VAL:CG1	2:B:90:LYS:CD	0.45	2.91
2:B:115:GLU:HB2	2:B:116:PRO:CD	0.45	2.42
2:B:74:PHE:CE1	2:B:87:PHE:HB2	0.45	2.47
2:B:115:GLU:O	2:B:117:VAL:HG23	0.45	2.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:21:PHE:CE1	2:B:96:GLU:CB	0.45	3.00
1:A:427:VAL:HG23	2:B:112:VAL:HB	0.44	1.88
2:B:59:TYR:OH	2:B:104:ILE:CD1	0.44	2.66
2:B:72:PHE:CZ	2:B:74:PHE:CG	0.44	3.06
2:B:115:GLU:CB	2:B:116:PRO:CD	0.43	2.96
2:B:21:PHE:CZ	2:B:96:GLU:HB3	0.43	2.47
2:B:25:ASN:O	2:B:33:LEU:CD1	0.43	2.67
2:B:59:TYR:O	2:B:62:LEU:CD1	0.42	2.67
2:B:68:ASP:O	2:B:70:ASN:N	0.42	2.52
2:B:26:VAL:CG1	2:B:90:LYS:HD3	0.42	2.44
2:B:20:LYS:CA	2:B:38:MET:O	0.42	2.67
1:A:412:MET:CB	2:B:82:THR:HG22	0.42	2.44
2:B:25:ASN:O	2:B:33:LEU:CG	0.42	2.68
1:A:428:THR:HG22	1:A:428:THR:O	0.42	2.14
1:A:429:VAL:HG22	1:A:429:VAL:O	0.42	2.15
2:B:21:PHE:O	2:B:23:VAL:N	0.42	2.53
2:B:65:TYR:CD2	2:B:101:LEU:CD2	0.42	3.03
2:B:15:ASP:O	2:B:17:HIS:N	0.41	2.53
2:B:67:TYR:CE1	2:B:98:PHE:CD2	0.41	3.09
2:B:45:LEU:HD12	2:B:59:TYR:CE1	0.41	2.50
2:B:20:LYS:CB	2:B:38:MET:O	0.41	2.68
1:A:429:VAL:O	2:B:63:ARG:C	0.41	2.59
2:B:100:MET:O	2:B:103:GLU:N	0.41	2.52
2:B:60:LEU:HB2	2:B:110:ILE:CG2	0.41	2.46
1:A:427:VAL:CG2	2:B:112:VAL:HB	0.41	2.46
1:A:426:GLN:HB2	2:B:116:PRO:CD	0.41	2.46
2:B:120:ARG:O	2:B:122:ASN:N	0.41	2.54
2:B:74:PHE:CE1	2:B:87:PHE:CB	0.40	3.03
2:B:38:MET:HA	2:B:47:LEU:CD1	0.40	2.46
2:B:40:LEU:HD13	2:B:100:MET:CE	0.40	2.46

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR 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	A	20/22 (91%)	11 (55%)	6 (30%)	3 (15%)	1 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	127/129 (98%)	87 (69%)	26 (20%)	14 (11%)	1	8
All	All	147/151 (97%)	98 (67%)	32 (22%)	17 (12%)	1	7

All 17 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	B	41	THR
2	B	118	VAL
2	B	80	CYS
2	B	35	SER
1	A	414	VAL
2	B	16	ASN
2	B	81	GLN
2	B	121	ASN
2	B	59	TYR
2	B	128	GLU
1	A	411	GLN
2	B	69	SER
2	B	113	VAL
2	B	62	LEU
2	B	32	GLU
2	B	22	LYS
1	A	412	MET

6.3.2 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 PDB entries followed by that with respect to all NMR 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	A	20/20 (100%)	14 (70%)	6 (30%)	2	17
2	B	118/118 (100%)	79 (67%)	39 (33%)	1	12
All	All	138/138 (100%)	93 (67%)	45 (33%)	1	12

All 45 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	B	127	LEU
1	A	419	LYS
2	B	56	LYS
2	B	18	ARG
2	B	99	ASN
2	B	78	ARG
2	B	55	VAL
1	A	427	VAL
2	B	11	ASP
2	B	98	PHE
2	B	67	TYR
2	B	54	SER
2	B	35	SER
2	B	51	LYS
2	B	50	ARG
1	A	426	GLN
2	B	109	SER
2	B	107	ASN
2	B	64	ARG
2	B	119	GLU
1	A	425	ARG
2	B	40	LEU
2	B	29	ASP
2	B	32	GLU
1	A	410	SER
2	B	60	LEU
2	B	93	ARG
1	A	420	SER
2	B	8	MET
2	B	131	ARG
2	B	10	SER
2	B	74	PHE
2	B	128	GLU
2	B	43	THR
2	B	108	ASN
2	B	126	GLU
2	B	49	THR
2	B	20	LYS
2	B	118	VAL
2	B	80	CYS
2	B	63	ARG
2	B	84	GLN
2	B	59	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	65	TYR
2	B	103	GLU

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided