wwPDB NMR Structure Validation Summary Report (i)

Oct 16, 2021 – 06:23 PM EDT

PDB ID	:	1PLO
Title	:	TRANSFORMING GROWTH FACTOR-BETA TYPE II RECEPTOR EXTRACELLULAR DOMAIN
Authors	:	Deep, S.; Walker III, K.P.; Shu, Z.; Hinck, A.P.
Deposited on	:	2003-06-08

This is a wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

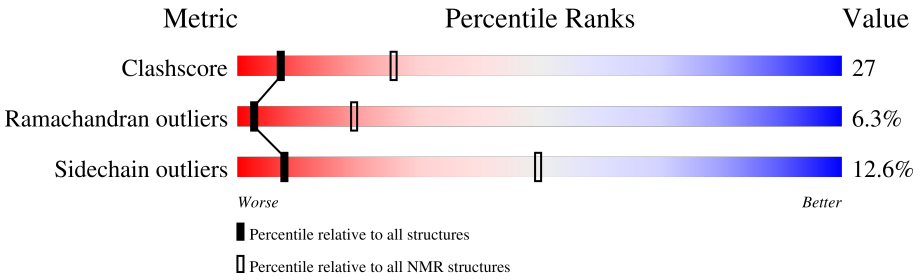
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	122	43% 38% 5% 15%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations, lowest energy.*

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:24-A:127 (104)	0.62	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	7, 8, 10
2	1, 4, 6
3	3, 9
Single-model clusters	2; 5

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1853 atoms, of which 897 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TGF-beta receptor type II.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	122	1853	590	897	156	195	15	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	ASN	engineered mutation	UNP P37173

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: TGF-beta receptor type II

Chain A: 43% 38% 5% 15%

V15 T16 D17 N18 A19 G20 A21 V22 K23 F24 L27 C28 K29 F30 C31 D32 V33 R34 C38 D39 N40 Q41 K42 S43 C44 V60 A63 V64 W65 R66 K67 N68 D69 E70 N71 I72 V77 C78 H79 D80 L83 P84 Y85 H86 D87 F88 I89 L90 C98 I99 M100 K101 E102

K103 K104 K105 P106 G107 E108 T109 F110 F111 M112 C113 D118 E119 C120 N121 I124 I125 F126 S127 E128 E129 Y130 N131 T132 S133 N134 P135 D136

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 9. Colouring as in section 4.1 above.

• Molecule 1: TGF-beta receptor type II

Chain A: 43% 30% 12% 15%

V15 T16 D17 N18 A19 G20 A21 V22 K23 F24 C28 K29 F30 C31 D32 V33 R34 C38 D39 N40 Q41 K42 S43 C44 C48 S49 I50 V60 A63 V64 W65 R66 K67 N68 D69 E70 N71 I72 T73 L74 V77 C78 H79 D80 Y85 H86 D87 F88 I89 L90 E91 D92

K97 K101 E102 K103 K104 K105 P106 G107 E108 T109 F110 F111 N121 I124 I125 F126 S127 E128 E129 Y130 N131 T132 S133 N134 P135 D136

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *substructure distance geometry, full structure distance geometry-simulated annealing; torsion angle dynamics.*

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with favorable non-bond energy, structures with the least restraint violations, structures with the lowest energy.*

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

Software name	Classification	Version
XPLOR NIH	refinement	1.06

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.0±0.0
All	All	0	20

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	34	ARG	Sidechain	10
1	A	66	ARG	Sidechain	10

6.2 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 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	821	778	778	43±7
All	All	8210	7780	7774	426

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 27.

5 of 281 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:GLU:OE1	1:A:109:THR:N	1.31	1.61	9	3
1:A:38:CYS:C	1:A:39:ASP:OD1	1.20	1.80	5	2
1:A:108:GLU:OE1	1:A:108:GLU:CA	1.10	1.98	7	3
1:A:108:GLU:HA	1:A:108:GLU:OE1	1.09	1.41	6	1
1:A:108:GLU:CD	1:A:109:THR:H	1.07	1.52	9	2

6.3 Torsion angles (i)

6.3.1 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 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	104/122 (85%)	86±3 (82±3%)	12±2 (11±2%)	7±1 (6±1%)	3	19
All	All	1040/1220 (85%)	857 (82%)	117 (11%)	66 (6%)	3	19

5 of 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	102	GLU	8
1	A	41	GLN	6
1	A	118	ASP	5
1	A	89	ILE	5
1	A	107	GLY	5

6.3.2 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 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	100/115 (87%)	87±3 (87±3%)	13±3 (13±3%)	8	50
All	All	1000/1150 (87%)	874 (87%)	126 (13%)	8	50

5 of 47 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	98	CYS	6
1	A	105	LYS	6
1	A	44	CYS	5
1	A	83	LEU	5
1	A	86	HIS	5

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 monosaccharides 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 (i)

No chemical shift data were provided