



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2N97
Title : DD homodimer
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Deposited on : 2015-11-07

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

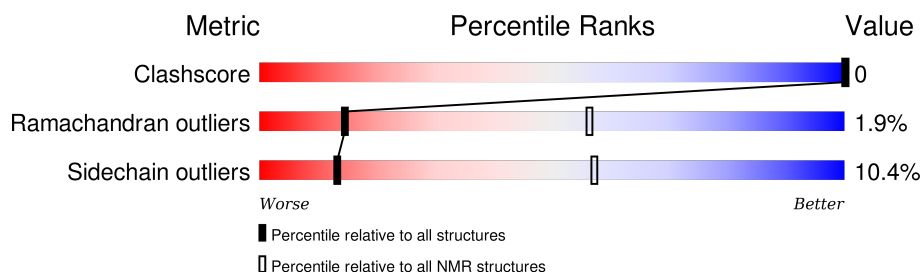
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 39%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	98	 79% 7% 10% •
1	B	98	 81% 7% 8% •

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:335-A:418, B:334-B:419 (170)	0.29	2

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 1 single-model cluster was found.

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

3 Entry composition [i](#)

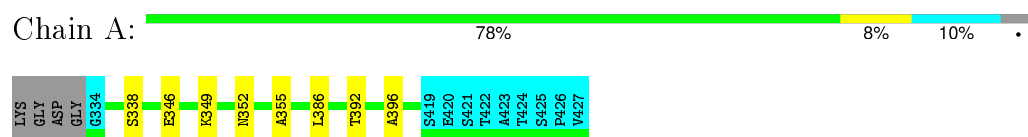
There is only 1 type of molecule in this entry. The entry contains 2826 atoms, of which 1398 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor necrosis factor receptor superfamily member 16.

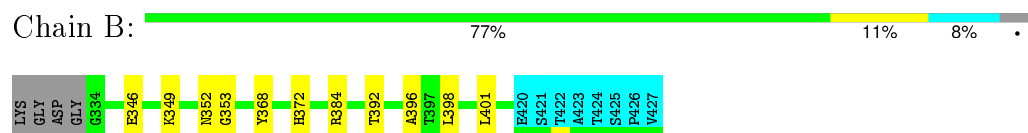
Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1413	444	699	126	142	2	
1	B	94	Total	C	H	N	O	S	0
			1413	444	699	126	142	2	

4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Tumor necrosis factor receptor superfamily member 16

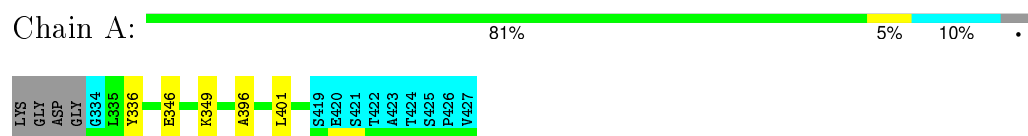


- Molecule 1: Tumor necrosis factor receptor superfamily member 16

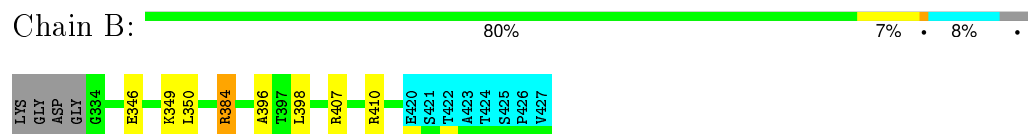


4.2.3 Score per residue for model 3

- Molecule 1: Tumor necrosis factor receptor superfamily member 16

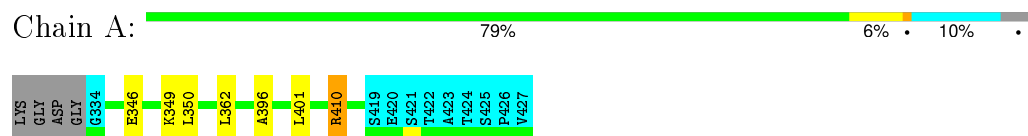


- Molecule 1: Tumor necrosis factor receptor superfamily member 16

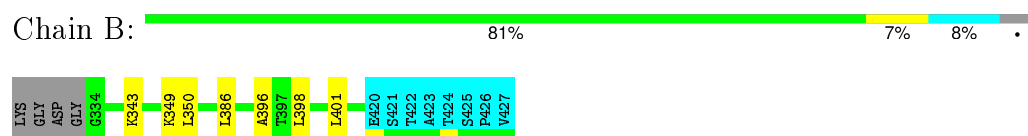


4.2.4 Score per residue for model 4

- Molecule 1: Tumor necrosis factor receptor superfamily member 16

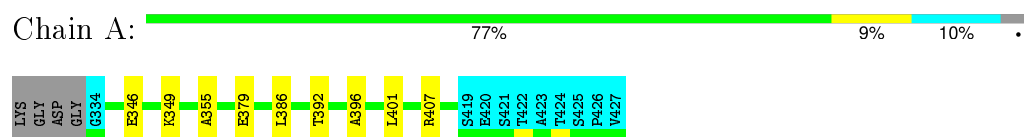


- Molecule 1: Tumor necrosis factor receptor superfamily member 16

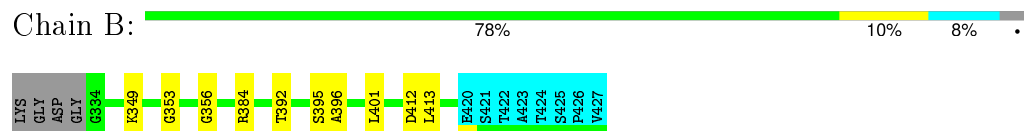


4.2.8 Score per residue for model 8

- Molecule 1: Tumor necrosis factor receptor superfamily member 16

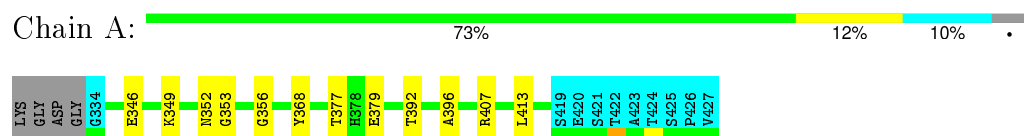


- Molecule 1: Tumor necrosis factor receptor superfamily member 16

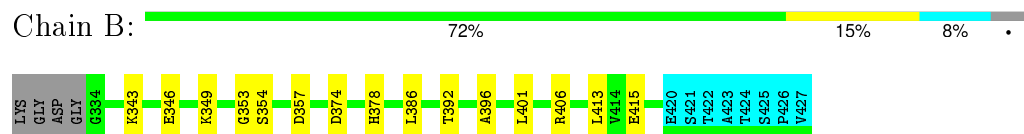


4.2.9 Score per residue for model 9

- Molecule 1: Tumor necrosis factor receptor superfamily member 16

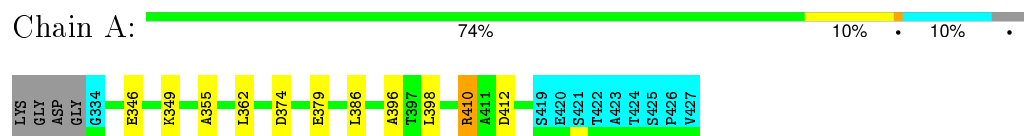


- Molecule 1: Tumor necrosis factor receptor superfamily member 16

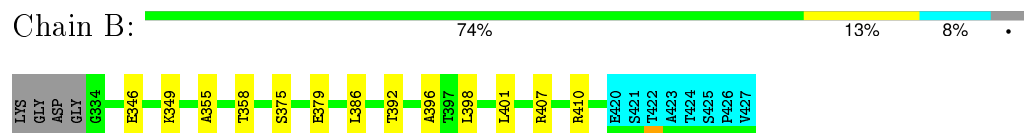


4.2.10 Score per residue for model 10

- Molecule 1: Tumor necrosis factor receptor superfamily member 16



- Molecule 1: Tumor necrosis factor receptor superfamily member 16



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
AMBER	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2n97_cs.str
Number of chemical shift lists	1
Total number of shifts	999
Number of shifts mapped to atoms	999
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	39%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 (average) 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	0.70±0.00	0±0/664 (0.0±0.0%)	0.93±0.01	0±0/905 (0.0±0.1%)
1	B	0.69±0.01	0±0/674 (0.0±0.0%)	0.94±0.02	1±1/918 (0.1±0.1%)
All	All	0.70	0/13380 (0.0%)	0.93	12/18230 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	384	ARG	NE-CZ-NH1	7.45	124.03	120.30	3	2
1	B	410	ARG	NE-CZ-NH1	6.45	123.53	120.30	7	3
1	B	407	ARG	NE-CZ-NH1	6.29	123.45	120.30	3	2
1	A	410	ARG	NE-CZ-NH1	5.62	123.11	120.30	6	3
1	B	384	ARG	NE-CZ-NH2	-5.61	117.50	120.30	2	1
1	B	344	ARG	NE-CZ-NH1	5.27	122.94	120.30	6	1

There are no chirality outliers.

There are no planarity outliers.

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	650	640	640	0±0
1	B	660	648	647	0±0
All	All	13100	12880	12870	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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:377:THR:HG23	1:B:357:ASP:HB3	0.45	1.88	9	1

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	84/98 (86%)	81±1 (96±1%)	2±1 (2±1%)	2±1 (2±1%)	15	58
1	B	85/98 (87%)	80±1 (95±2%)	3±1 (3±1%)	2±1 (2±1%)	14	55
All	All	1690/1960 (86%)	1610 (95%)	48 (3%)	32 (2%)	14	56

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	396	ALA	10
1	A	396	ALA	10
1	B	353	GLY	3
1	A	355	ALA	3
1	A	353	GLY	1
1	B	357	ASP	1
1	A	356	GLY	1
1	B	354	SER	1
1	B	356	GLY	1
1	B	355	ALA	1

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	68/78 (87%)	61±2 (90±3%)	7±2 (10±3%)	15	59
1	B	69/78 (88%)	61±2 (89±3%)	8±2 (11±3%)	12	55
All	All	1370/1560 (88%)	1227 (90%)	143 (10%)	13	57

All 50 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	B	349	LYS	10
1	A	349	LYS	10
1	B	401	LEU	8
1	B	398	LEU	8
1	A	379	GLU	7
1	A	401	LEU	7
1	A	346	GLU	7
1	B	386	LEU	7
1	B	392	THR	5
1	B	379	GLU	5
1	A	386	LEU	5
1	B	346	GLU	4
1	A	392	THR	4
1	B	413	LEU	3
1	B	343	LYS	3
1	B	352	ASN	3
1	A	407	ARG	3
1	A	352	ASN	2
1	B	384	ARG	2
1	A	374	ASP	2
1	A	362	LEU	2
1	A	413	LEU	2
1	B	350	LEU	2
1	A	384	ARG	2
1	B	368	TYR	2
1	A	410	ARG	2
1	B	406	ARG	2
1	A	398	LEU	2
1	A	406	ARG	1
1	B	358	THR	1
1	B	360	ARG	1
1	A	336	TYR	1
1	B	399	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	360	ARG	1
1	B	357	ASP	1
1	B	378	HIS	1
1	B	374	ASP	1
1	A	405	LEU	1
1	A	368	TYR	1
1	B	405	LEU	1
1	B	412	ASP	1
1	A	343	LYS	1
1	B	375	SER	1
1	B	395	SER	1
1	B	415	GLU	1
1	A	338	SER	1
1	B	372	HIS	1
1	A	412	ASP	1
1	A	350	LEU	1
1	B	354	SER	1

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 39% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: 2n97_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	999
Number of shifts mapped to atoms	999
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	97	-0.04 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	90	0.76 ± 0.08	Should be applied
$^{13}\text{C}'$	0	—	—
^{15}N	93	0.63 ± 0.43	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 39%, i.e. 785 atoms were assigned a chemical shift out of a possible 2035. 16 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	321/834 (38%)	158/332 (48%)	83/340 (24%)	80/162 (49%)
Sidechain	431/1061 (41%)	263/620 (42%)	163/393 (41%)	5/48 (10%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	33/140 (24%)	18/74 (24%)	13/56 (23%)	2/10 (20%)
Overall	785/2035 (39%)	439/1026 (43%)	259/789 (33%)	87/220 (40%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 858 atoms were assigned a chemical shift out of a possible 2200. 17 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	358/920 (39%)	176/366 (48%)	93/376 (25%)	89/178 (50%)
Sidechain	467/1140 (41%)	285/666 (43%)	177/426 (42%)	5/48 (10%)
Aromatic	33/140 (24%)	18/74 (24%)	13/56 (23%)	2/10 (20%)
Overall	858/2200 (39%)	479/1106 (43%)	283/858 (33%)	96/236 (41%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	382	PRO	HB3	-0.18	3.81 – 0.21	-6.1
1	A	396	ALA	HB3	-0.12	2.61 – 0.11	-5.9
1	A	396	ALA	HB1	-0.12	2.61 – 0.11	-5.9
1	A	396	ALA	HB2	-0.12	2.61 – 0.11	-5.9
1	A	360	ARG	HG2	0.04	2.92 – 0.22	-5.7
1	A	360	ARG	HG3	0.07	3.00 – 0.10	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

