wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2PTL
Title	:	THREE-DIMENSIONAL SOLUTION STRUCTURE OF AN IMMUNOGLOBULIN LIGHT CHAIN-BINDING DOMAIN OF PROTEIN L. COMPARISON WITH THE IGG-BINDING DOMAINS OF PROTEIN G
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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
http://wwpdb.org/validation/2016/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:

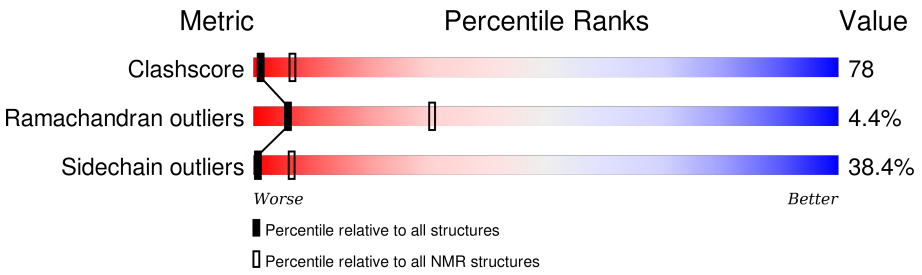
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	78	8% 63% 8% 22%

2 Ensemble composition and analysis (i)

This entry contains 21 models. Model 4 is the overall representative, medoid model (most similar to other models).

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:18-A:78 (61)	0.53	4

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 17, 18, 19, 20, 21
2	14, 16
Single-model clusters	15

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1172 atoms, of which 567 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN L.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	78	1172	376	567	92	137	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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: PROTEIN L

Chain A: 8% 63% 8% 22%

E1 N2 K3 E4 E5 T6 P7 E8 T9 P10 E11 T12 D13 S14 E15 E16 E17 V18 T19 I20 K21 A22 N23 L24 I25 F26 A27 N28 G29 S30 T31 Q32 T33 A34 E35 F36 K37 G38 T39 F40 E41 K42 A43 T44 S45 E46 A47 Y48 A49 Y50 A51 D52 T53 L54 K55 K56 D57 N58 G59 E60

Y61 T62 V63 D64 V65 A66 D67 K68 G69 Y70 T71 L72 N73 I74 K75 F76 A77 G78

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

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: PROTEIN L

Chain A: 21% 40% 18% 22%

E1 N2 K3 E4 E5 T6 P7 E8 T9 P10 E11 T12 D13 S14 E15 E16 E17 V18 T19 I20 N23 L24 I25 F26 A27 N28 G29 S30 T31 Q32 T33 A34 E35 F36 K37 G38 T39 F40 E41 K42 A43 T44 S45 E46 A47 Y48 A51 D52 T53 L54 K55 N58 G59 E60 Y61 T62 V63

D64 V65 A66 D67 K68 G69 Y70 T71 L72 N73 I74 K75 F76 A77 G78

5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 21 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	

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 (i)

6.1 Standard geometry (i)

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 (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	467	454	454	72±9
All	All	9807	9534	9534	1517

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 78.

5 of 562 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ALA:HB3	1:A:34:ALA:HB3	1.02	1.32	2	4
1:A:61:TYR:CD1	1:A:74:ILE:HG23	1.02	1.89	16	11
1:A:20:ILE:HD12	1:A:70:TYR:CE1	1.01	1.90	18	20
1:A:20:ILE:HG21	1:A:43:ALA:CB	0.99	1.87	16	19
1:A:54:LEU:HD21	1:A:76:PHE:CZ	0.96	1.95	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	60/78 (77%)	45±3 (75±5%)	12±3 (20±5%)	3±1 (4±2%)	6 30
All	All	1260/1638 (77%)	948 (75%)	257 (20%)	55 (4%)	6 30

5 of 14 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	39	THR	13
1	A	55	LYS	10
1	A	77	ALA	7
1	A	29	GLY	5
1	A	18	VAL	4

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	47/64 (73%)	29±2 (62±5%)	18±2 (38±5%)	1 6
All	All	987/1344 (73%)	608 (62%)	379 (38%)	1 6

5 of 42 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	36	PHE	21
1	A	70	TYR	20
1	A	72	LEU	20
1	A	48	TYR	19
1	A	37	LYS	16

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 (i)

No chemical shift data were provided