Full wwPDB NMR Structure Validation Report (i)

Feb 9, 2022 – 08:11 AM EST

PDB ID	:	1DGQ
Title	:	NMR SOLUTION STRUCTURE OF THE INSERTED DOMAIN OF HUMAN LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1
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Deposited on	:	1999-11-24

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 (i) symbol.

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

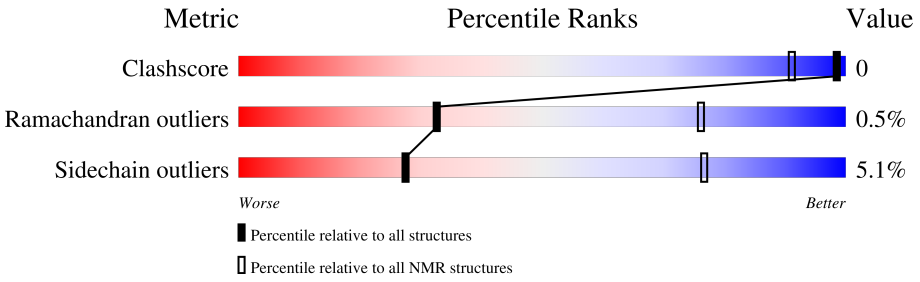
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	188	84% 5% 12%

2 Ensemble composition and analysis (i)

This entry contains 22 models. Model 13 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:130-A:161, A:166-A:299 (166)	0.19	13

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 10, 11, 12, 19, 20, 21
2	7, 13, 14, 17, 18
3	2, 6, 9, 22
4	5, 8, 15
Single-model clusters	4; 16

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3029 atoms, of which 1519 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	188	3029	978	1519	239	288	5	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	GLU	conflict	UNP P20701
A	125	ALA	CYS	conflict	UNP P20701
A	126	SER	ILE	conflict	UNP P20701
A	189	TRP	ARG	conflict	UNP P20701

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: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 84% 5% 12%

M124 A125 S126 K127 G128 N129 S141 S162 N163 T164 S165 Y166 Y186 T208 K232 N247 R256 Y257 F285 T300 E301 L302 Q303 K304 K305 I306 Y307 V308 I309 E310 G311

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 80% 8% 12%

M124 A125 S126 K127 G128 N129 M140 S141 S162 N163 T164 S165 Y166 Q167 S174 Y186 T208 K232 N247 R256 Y257 T267 K268 S283 E284 F285 T300 E301 L302 Q303 K304 K305 I306 Y307 V308 I309 E310 G311

4.2.2 Score per residue for model 2

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

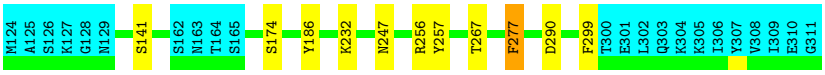
Chain A: 80% 8% 12%

M124 A125 S126 K127 G128 N129 K155 S162 N163 T164 S165 Y166 Y186 T208 F209 Y214 R221 K232 N247 R256 Y257 T267 S283 T291 F299 T300 E301 L302 Q303 K304 K305 I306 Y307 V308 I309 E310 G311

4.2.3 Score per residue for model 3

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 82% 5% • 12%



4.2.4 Score per residue for model 4

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 81% 6% • 12%

4.2.5 Score per residue for model 5

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 81% 7% 12%

4.2.6 Score per residue for model 6

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 79% 9% 12%

4.2.7 Score per residue for model 7

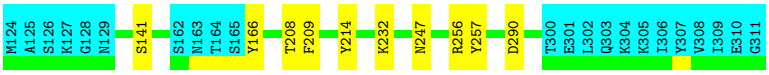
• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 81% 7% 12%

4.2.8 Score per residue for model 8

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

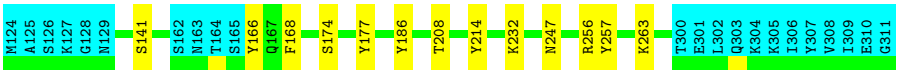
Chain A: 83% 5% 12%



4.2.9 Score per residue for model 9

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 81% 7% 12%



4.2.10 Score per residue for model 10

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 84% • 12%

4.2.11 Score per residue for model 11

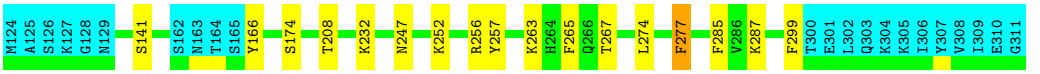
• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 80% 8% 12%

4.2.12 Score per residue for model 12

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 79% 9% • 12%



4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 81% 7% 12%

4.2.14 Score per residue for model 14

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 81% 7% 12%

4.2.15 Score per residue for model 15

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 82% 6% 12%

4.2.16 Score per residue for model 16

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 82% 6% 12%

4.2.17 Score per residue for model 17

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 81% 7% 12%

4.2.18 Score per residue for model 18

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 84% 5% 12%

4.2.19 Score per residue for model 19

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 79% 9% • 12%

4.2.20 Score per residue for model 20

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 81% 7% • 12%

4.2.21 Score per residue for model 21

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 82% 6% 12%

4.2.22 Score per residue for model 22

• Molecule 1: LEUKOCYTE FUNCTION ASSOCIATED ANTIGEN-1

Chain A: 82% 6% 12%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *TORSION ANGLE DYNAMICS SIMULATED ANNEALING.*

Of the 100 calculated structures, 22 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
DYANA	structure solution	1.5
Amber	structure solution	5.1
Amber	refinement	5.1

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	4.8±1.1
All	All	0	105

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	257	TYR	Sidechain	22
1	A	186	TYR	Sidechain	15
1	A	166	TYR	Sidechain	12
1	A	285	PHE	Sidechain	11
1	A	299	PHE	Sidechain	10
1	A	209	PHE	Sidechain	9
1	A	147	PHE	Sidechain	6
1	A	214	TYR	Sidechain	5
1	A	277	PHE	Sidechain	5
1	A	221	ARG	Sidechain	4
1	A	153	PHE	Sidechain	2
1	A	227	ARG	Sidechain	2
1	A	136	PHE	Sidechain	1
1	A	168	PHE	Sidechain	1

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	1343	1346	1346	0±0
All	All	29546	29612	29612	3

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:136:PHE:CE2	1:A:147:PHE:CE1	0.43	3.06	4	1
1:A:265:PHE:CZ	1:A:274:LEU:HD21	0.42	2.50	12	1
1:A:196:LEU:O	1:A:199:VAL:HG23	0.40	2.16	6	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	166/188 (88%)	150±2 (91±1%)	15±2 (9±1%)	1±1 (0±0%)	32 76
All	All	3652/4136 (88%)	3311 (91%)	323 (9%)	18 (0%)	32 76

All 3 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	174	SER	10
1	A	290	ASP	5
1	A	265	PHE	3

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	147/166 (89%)	139±2 (95±1%)	8±2 (5±1%)	27 77
All	All	3234/3652 (89%)	3068 (95%)	166 (5%)	27 77

All 30 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	232	LYS	22
1	A	247	ASN	22
1	A	256	ARG	22
1	A	141	SER	17
1	A	208	THR	16
1	A	283	SER	9
1	A	267	THR	8
1	A	140	MET	6
1	A	263	LYS	6
1	A	277	PHE	5
1	A	160	LYS	4
1	A	268	LYS	3
1	A	252	LYS	3
1	A	289	LEU	3
1	A	167	GLN	2
1	A	266	GLN	2
1	A	177	TYR	2
1	A	287	LYS	2
1	A	155	LYS	1
1	A	291	THR	1
1	A	136	PHE	1
1	A	148	GLN	1
1	A	294	LYS	1
1	A	143	GLN	1
1	A	239	ASP	1
1	A	188	LYS	1
1	A	222	GLU	1
1	A	271	GLN	1
1	A	241	GLU	1
1	A	184	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 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