

# Full wwPDB NMR Structure Validation Report (i)

### Feb 13, 2022 - 09:05 PM EST

PDB ID	:	1I98
Title	:	NMR ENSEMBLE OF ION-SELECTIVE LIGAND D18 FOR PLATELET
		INTEGRIN ALPHAIIB-BETA3
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Deposited on	:	2001-03-18

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 (1)) were used in the production of this report:

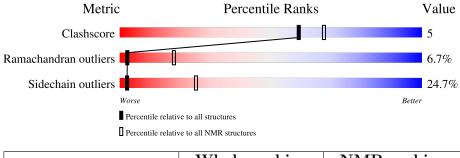
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${f NMR}  { m archive} \ (\#{ m Entries})$
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	А	13	31%	54%	15%



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# 2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 10 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:2-A:12 (11)	1.10	10		

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	2, 4, 6, 7, 10, 11, 12, 13
2	1, 8, 14
3	3, 5
Single-model clusters	9; 15



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# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 204 atoms, of which 98 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called ION-SELECTIVE LIGAND D18.

Mol	Chain	Residues		I	Aton	ıs			Trace
1	А	13	Total 204	C 65	Н 98	N 24	0 15	S 2	1



# 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: ION-SELECTIVE LIGAND D18

Chain A:	31%	54%	15%
ACB1 C2 V4 V4 L5 R6 W9 R10	NH213		

# 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: ION-SELECTIVE LIGAND D18



## 4.2.2 Score per residue for model 2





### 4.2.3 Score per residue for model 3

• Molecule 1: ION-SELECTIVE LIGAND D18



#### 4.2.4 Score per residue for model 4

• Molecule 1: ION-SELECTIVE LIGAND D18



#### 4.2.5 Score per residue for model 5

• Molecule 1: ION-SELECTIVE LIGAND D18

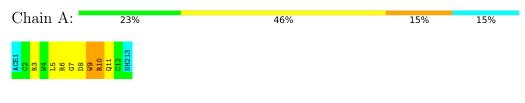
Chain A:	31%	38%	15%	15%
ACE1 C2 V4 V4 V4 V5 V4 V4 V4 V6 V6 V7 V6 V9 V9 V10 V13				

#### 4.2.6 Score per residue for model 6

#### • Molecule 1: ION-SELECTIVE LIGAND D18



#### 4.2.7 Score per residue for model 7





### 4.2.8 Score per residue for model 8

• Molecule 1: ION-SELECTIVE LIGAND D18



#### 4.2.9 Score per residue for model 9

• Molecule 1: ION-SELECTIVE LIGAND D18

Chain A:	15%	46%	15%	8%	15%
ACE1 C2 W4 L5 R6 R6 G7 D8	W9 R10 Q11 C12 NH213				

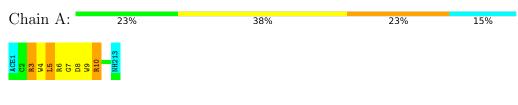
- 4.2.10 Score per residue for model 10 (medoid)
- Molecule 1: ION-SELECTIVE LIGAND D18

Chain A:	54%	15%	15%	15%
ACE1 C2 R3 W4 W5 R6 R1 R10 N1213				

- 4.2.11 Score per residue for model 11
- Molecule 1: ION-SELECTIVE LIGAND D18

Chain A:	46%	38%	15%
ACE1 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2			

#### 4.2.12 Score per residue for model 12





## 4.2.13 Score per residue for model 13

• Molecule 1: ION-SELECTIVE LIGAND D18



### 4.2.14 Score per residue for model 14

• Molecule 1: ION-SELECTIVE LIGAND D18



## 4.2.15 Score per residue for model 15

Chain A:	38%	38%	8%	15%
ACB1 C2 R3 W4 L5 R6 R6 R9 R10 R10				



# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *RESTRAINED MOLECULAR DYNAMICS* AND CHEMICAL SHIFT REFINEMENT..

Of the 200 calculated structures, 15 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
X-PLOR	refinement	3.8.5.1 (CHEM.SHIFT.MODULE)

No chemical shift data was provided.



# 6 Model quality (i)

# 6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE

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	А	$0.0{\pm}0.0$	$3.0{\pm}0.0$
All	All	0	45

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	А	3	ARG	Sidechain	15
1	А	6	ARG	Sidechain	15
1	А	10	ARG	Sidechain	15

# 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	А	102	93	93	1±1
All	All	1530	1395	1395	14

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 5.

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



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Mod	lels
Atom-1	Atom-2 Clash(A)		Distance(A)	Worst	Total
1:A:5:LEU:HD13	1:A:5:LEU:H	0.78	1.38	10	1
1:A:5:LEU:HD13	1:A:5:LEU:N	0.69	2.02	10	1
1:A:3:ARG:O	1:A:4:TRP:CD1	0.50	2.65	12	2
1:A:5:LEU:N	1:A:5:LEU:CD1	0.47	2.72	10	1
1:A:4:TRP:CZ3	1:A:5:LEU:HD21	0.46	2.45	9	1
1:A:5:LEU:H	1:A:5:LEU:CD1	0.43	2.11	10	1
1:A:3:ARG:O	1:A:4:TRP:CG	0.42	2.72	13	1
1:A:7:GLY:O	1:A:8:ASP:CG	0.42	2.58	12	1
1:A:5:LEU:CD2	1:A:5:LEU:C	0.41	2.88	10	1
1:A:7:GLY:O	1:A:9:TRP:N	0.41	2.54	5	2
1:A:5:LEU:HD21	1:A:11:GLN:CG	0.41	2.46	6	1
1:A:5:LEU:O	1:A:5:LEU:HG	0.40	2.16	12	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	Analysed Favoured Allowed Outliers		Outliers	Pe	rcentiles
1	А	11/13~(85%)	$7\pm2~(64\pm15\%)$	$3\pm2~(29\pm17\%)$	$1\pm1~(7\pm6\%)$	4	2 18
All	All	165/195~(85%)	106 (64%)	48 (29%)	11 (7%)	4	2 18

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	2	CYS	8
1	А	11	GLN	1
1	А	8	ASP	1
1	А	5	LEU	1

### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.



Mol	Chain	Chain Analysed Rotamer		Outliers	P	erce	entiles
1	А	10/10~(100%)	$8\pm1$ (75 $\pm13\%$ )	$2\pm1 (25\pm13\%)$		2	25
All	All	150/150~(100%)	113 (75%)	37~(25%)		2	25

All 9 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	А	9	TRP	10
1	А	5	LEU	6
1	А	4	TRP	5
1	А	6	ARG	4
1	А	8	ASP	4
1	А	10	ARG	3
1	А	11	GLN	2
1	А	3	ARG	2
1	А	12	CYS	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

