Full wwPDB NMR Structure Validation Report (i)

Dec 13, 2023 – 06:26 PM EST

PDB ID	:	2JOD
BMRB ID	:	15166
Title	:	Pac1-Rshort N-terminal EC domain Pacap(6-38) complex
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Deposited on	:	2007-03-07

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

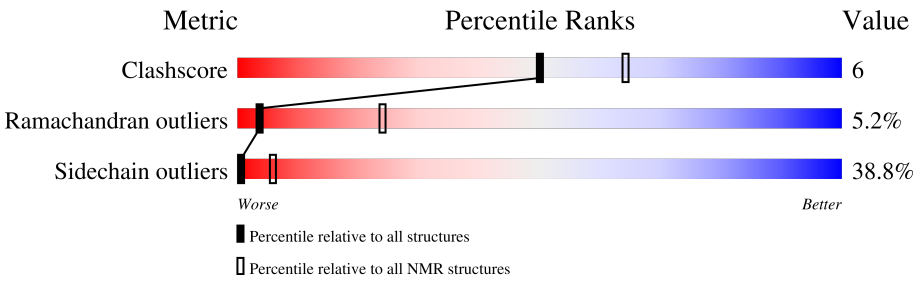
SOFTWARE-VERSIONS INFOmissingINFO

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 is 52%.

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	106	59% 28% 12%
2	B	33	45% 45% 9%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2180 atoms, of which 1062 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pituitary adenylate cyclase-activating polypeptide type I receptor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	106	1587	521	753	136	164	13	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	cloning artifact	UNP P41586
A	18	GLY	-	cloning artifact	UNP P41586
A	19	SER	-	cloning artifact	UNP P41586
A	20	MET	-	cloning artifact	UNP P41586
A	21	ALA	-	cloning artifact	UNP P41586
A	25	GLY	CYS	engineered mutation	UNP P41586
A	?	-	VAL	deletion	UNP P41586
A	?	-	TRP	deletion	UNP P41586
A	?	-	GLU	deletion	UNP P41586
A	?	-	THR	deletion	UNP P41586
A	?	-	GLU	deletion	UNP P41586
A	?	-	THR	deletion	UNP P41586
A	?	-	ILE	deletion	UNP P41586
A	?	-	GLY	deletion	UNP P41586
A	?	-	GLU	deletion	UNP P41586
A	?	-	SER	deletion	UNP P41586
A	?	-	ASP	deletion	UNP P41586
A	?	-	PHE	deletion	UNP P41586
A	?	-	GLY	deletion	UNP P41586
A	?	-	ASP	deletion	UNP P41586
A	?	-	SER	deletion	UNP P41586
A	?	-	ASN	deletion	UNP P41586
A	?	-	SER	deletion	UNP P41586
A	?	-	LEU	deletion	UNP P41586
A	?	-	ASP	deletion	UNP P41586
A	?	-	LEU	deletion	UNP P41586
A	?	-	SER	deletion	UNP P41586

- Molecule 2 is a protein called Pituitary adenylate cyclase-activating polypeptide.

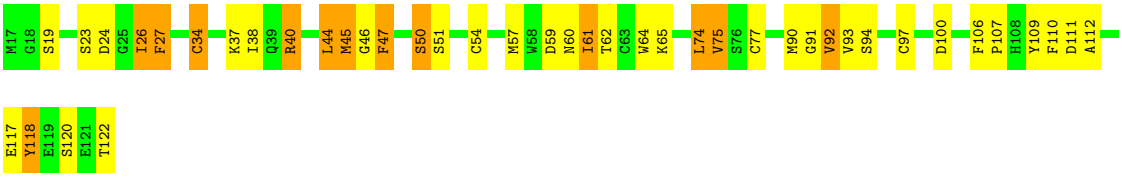
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	33	593	182	309	55	46	1	0

4 Residue-property plots (i)

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: Pituitary adenylate cyclase-activating polypeptide type I receptor

Chain A: 59% 28% 12%



• Molecule 2: Pituitary adenylate cyclase-activating polypeptide

Chain B: 45% 45% 9%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 300 calculated structures, 1 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
CNS	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	975
Number of shifts mapped to atoms	975
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	52%

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	834	753	750	10
2	B	284	309	306	4
All	All	1118	1062	1056	13

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:75:VAL:O	1:A:92:VAL:HA	0.62	1.95
1:A:62:THR:HB	1:A:90:MET:O	0.55	2.01
1:A:107:PRO:HA	2:B:19:VAL:HG13	0.53	1.80
1:A:74:LEU:HD23	1:A:92:VAL:CG2	0.49	2.38
2:B:10:TYR:O	2:B:14:ARG:HG2	0.48	2.09
2:B:35:VAL:O	2:B:35:VAL:HG13	0.48	2.09
2:B:23:LEU:O	2:B:27:LEU:HB2	0.47	2.09
1:A:40:ARG:O	1:A:44:LEU:HB3	0.46	2.10
1:A:59:ASP:HB2	1:A:64:TRP:HE1	0.43	1.72
1:A:34:CYS:O	1:A:38:ILE:HG13	0.42	2.15
1:A:45:MET:HB3	1:A:47:PHE:CE2	0.41	2.49
1:A:47:PHE:HB3	1:A:51:SER:O	0.41	2.14
1:A:26:ILE:C	1:A:27:PHE:CD1	0.41	2.95

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	104/106 (98%)	75 (72%)	23 (22%)	6 (6%)	3 21
2	B	31/33 (94%)	25 (81%)	5 (16%)	1 (3%)	7 38
All	All	135/139 (97%)	100 (74%)	28 (21%)	7 (5%)	4 24

All 7 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	46	GLY
1	A	50	SER
1	A	61	ILE
1	A	91	GLY
1	A	112	ALA
1	A	118	TYR
2	B	28	GLY

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	92/92 (100%)	59 (64%)	33 (36%)	1 8
2	B	29/29 (100%)	15 (52%)	14 (48%)	0 1
All	All	121/121 (100%)	74 (61%)	47 (39%)	0 6

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

Mol	Chain	Res	Type
1	A	19	SER
1	A	23	SER
1	A	24	ASP
1	A	26	ILE
1	A	27	PHE
1	A	34	CYS
1	A	37	LYS
1	A	40	ARG
1	A	44	LEU
1	A	45	MET
1	A	47	PHE
1	A	50	SER
1	A	54	CYS
1	A	57	MET
1	A	60	ASN
1	A	61	ILE
1	A	65	LYS
1	A	74	LEU
1	A	75	VAL
1	A	77	CYS
1	A	92	VAL
1	A	93	VAL
1	A	94	SER
1	A	97	CYS
1	A	100	ASP
1	A	106	PHE
1	A	109	TYR
1	A	110	PHE
1	A	111	ASP
1	A	117	GLU
1	A	118	TYR
1	A	120	SER
1	A	122	THR
2	B	7	THR
2	B	9	SER
2	B	10	TYR
2	B	12	ARG
2	B	17	MET
2	B	19	VAL
2	B	20	LYS
2	B	21	LYS
2	B	22	TYR
2	B	23	LEU

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Mol	Chain	Res	Type
2	B	29	LYS
2	B	30	ARG
2	B	36	LYS
2	B	38	LYS

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)

The completeness of assignment taking into account all chemical shift lists is 52% for the well-defined parts and 52% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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	975
Number of shifts mapped to atoms	975
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	97	-0.26 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	89	0.09 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	79	0.47 ± 0.53	None needed (< 0.5 ppm)
^{15}N	78	1.00 ± 0.25	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 52%, i.e. 975 atoms were assigned a chemical shift out of a possible 1866. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	433/691 (63%)	179/281 (64%)	176/278 (63%)	78/132 (59%)
Sidechain	451/984 (46%)	285/633 (45%)	164/308 (53%)	2/43 (5%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	91/191 (48%)	48/94 (51%)	40/91 (44%)	3/6 (50%)
Overall	975/1866 (52%)	512/1008 (51%)	380/677 (56%)	83/181 (46%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 975 atoms were assigned a chemical shift out of a possible 1866. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	433/691 (63%)	179/281 (64%)	176/278 (63%)	78/132 (59%)
Sidechain	451/984 (46%)	285/633 (45%)	164/308 (53%)	2/43 (5%)
Aromatic	91/191 (48%)	48/94 (51%)	40/91 (44%)	3/6 (50%)
Overall	975/1866 (52%)	512/1008 (51%)	380/677 (56%)	83/181 (46%)

7.1.4 Statistically unusual chemical shifts (i)

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.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	95	ARG	NE	115.32	76.53 – 92.65	19.1
1	A	95	ARG	HD3	-0.21	1.81 – 4.39	-12.8
1	A	95	ARG	HD2	1.74	1.97 – 4.26	-6.0

7.1.5 Random Coil Index (RCI) plots (i)

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

RCI
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
20:MET
25:GLY
30:GLU
34:CYS
38:ILE
42:ASN
46:GLY
50:SER
54:CYS
58:TRP
62:THR
66:PRO
70:GLY
74:LEU
78:PRO
86:PRO
90:MET
94:SER
98:THR
102:TRP
106:PHE
110:PHE
114:GLY
118:TYR
122:THR
Auth_seq_ID