



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 13, 2022 – 12:11 PM JST

PDB ID : 7D3W
Title : Non-specific and specific interactions work cooperatively to promote cytidine deamination catalyzed by APOBEC3A
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Deposited on : 2020-09-21

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

<https://www.wwpdb.org/validation/2017/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:

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	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

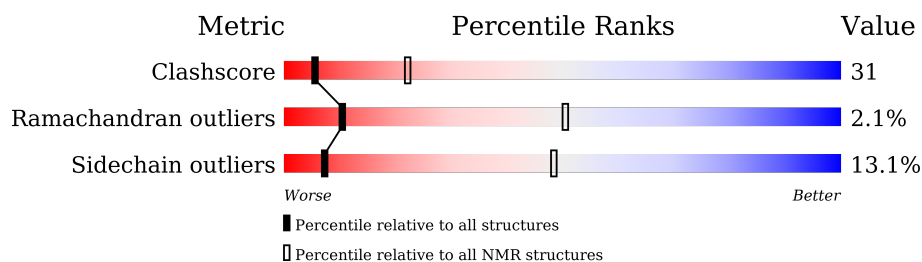
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 75%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	199	
2	B	10	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:12-A:59, A:70-A:101, A:106-A:197 (172)	0.47	17

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, 12, 13, 14, 15, 16, 17, 18, 19
2	9, 10, 20
Single-model clusters	11

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3490 atoms, of which 1664 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3A.

Mol	Chain	Residues	Atoms						Trace
1	A	199	Total	C	H	N	O	S	0
			3172	1029	1546	295	293	9	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ASN	LEU	engineered mutation	UNP P31941
A	64	SER	CYS	engineered mutation	UNP P31941
A	72	GLN	GLU	engineered mutation	UNP P31941
A	171	GLN	CYS	engineered mutation	UNP P31941

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	10	Total	C	H	N	O	P	0
			317	99	118	30	61	9	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

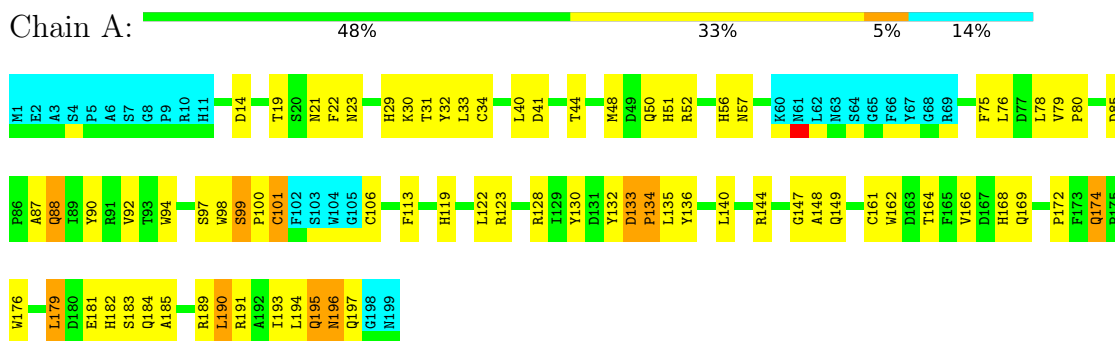
Mol	Chain	Residues	Atoms	
3	A	1	Total	Zn
			1	1

4 Residue-property plots

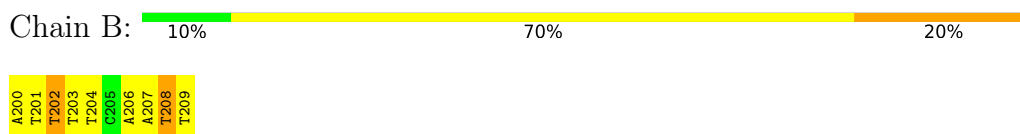
4.1 Average score per residue in the NMR ensemble

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: DNA dC->dU-editing enzyme APOBEC-3A



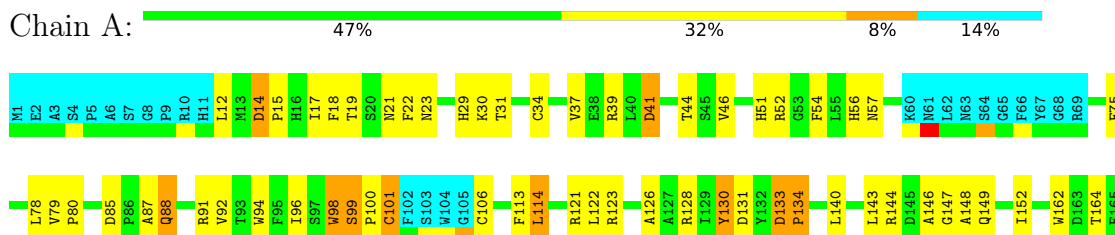
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

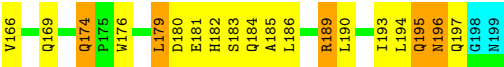


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

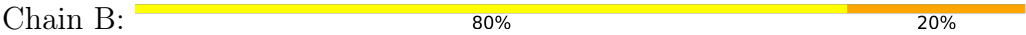
The representative model is number 17. Colouring as in section 4.1 above.

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





● Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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 NIH	structure calculation	
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	2276
Number of shifts mapped to atoms	2276
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

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: ZN

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	1.00±0.00	0±0/1460 (0.0± 0.0%)	0.91±0.00	0±0/1982 (0.0± 0.0%)
2	B	1.28±0.02	2±1/221 (0.9± 0.3%)	1.70±0.01	10±1/339 (2.8± 0.4%)
All	All	1.04	41/33620 (0.1%)	1.06	192/46420 (0.4%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	208	DT	C5-C7	5.99	1.53	1.50	5	19
2	B	201	DT	C5-C7	5.51	1.53	1.50	14	13
2	B	204	DT	C5-C7	5.17	1.53	1.50	5	4
2	B	209	DT	C5-C7	5.11	1.53	1.50	11	5

5 of 12 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
2	B	202	DT	C6-C5-C7	-6.18	119.19	122.90	7	20
2	B	201	DT	C6-C5-C7	-6.11	119.23	122.90	13	19
2	B	208	DT	C6-C5-C7	-6.09	119.25	122.90	5	20
2	B	209	DT	C6-C5-C7	-6.06	119.26	122.90	13	20
2	B	203	DT	C6-C5-C7	-5.87	119.38	122.90	7	20

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	1419	1357	1349	88±9
2	B	199	118	118	12±2
All	All	32380	29500	29340	1908

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 31.

5 of 709 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:TYR:O	1:A:158:PHE:CD1	1.23	1.90	20	1
1:A:158:PHE:CD1	1:A:159:LYS:N	1.02	2.25	20	1
1:A:179:LEU:H	1:A:179:LEU:HD22	0.94	1.21	2	15
1:A:162:TRP:HE1	1:A:168:HIS:CD2	0.92	1.82	12	5
1:A:40:LEU:HD13	1:A:40:LEU:O	0.91	1.64	3	1

6.3 Torsion angles

6.3.1 Protein backbone

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	172/199 (86%)	157±1 (91±1%)	11±1 (6±1%)	4±1 (2±1%)	10	50
All	All	3440/3980 (86%)	3146 (91%)	221 (6%)	73 (2%)	10	50

5 of 11 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	148	ALA	20
1	A	134	PRO	19

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Mol	Chain	Res	Type	Models (Total)
1	A	133	ASP	9
1	A	50	GLN	8
1	A	101	CYS	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	151/171 (88%)	131±2 (87±1%)	20±2 (13±1%)	7	48
All	All	3020/3420 (88%)	2625 (87%)	395 (13%)	7	48

5 of 69 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	88	GLN	20
1	A	174	GLN	20
1	A	189	ARG	20
1	A	190	LEU	20
1	A	195	GLN	20

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *A3A_shifts-nospecific_20200915.txt*

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	2276
Number of shifts mapped to atoms	2276
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	192	0.06 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	176	0.64 ± 0.15	Should be applied
$^{13}\text{C}'$	173	-0.02 ± 0.11	None needed (< 0.5 ppm)
^{15}N	181	-0.34 ± 0.31	None needed (< 0.5 ppm)

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 75%, i.e. 1815 atoms were assigned a chemical shift out of a possible 2412. 23 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	814/846 (96%)	328/337 (97%)	325/344 (94%)	161/165 (98%)
Sidechain	800/1113 (72%)	521/656 (79%)	273/396 (69%)	6/61 (10%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	118/265 (45%)	102/138 (74%)	14/106 (13%)	2/21 (10%)
Overall	1815/2412 (75%)	1034/1239 (83%)	612/916 (67%)	169/257 (66%)

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	94	TRP	HE1	5.58	12.85 – 7.35	-8.2
1	A	70	HIS	CE1	118.42	149.70 – 125.30	-7.8
1	A	66	PHE	CD2	124.86	137.34 – 125.84	-5.9
1	A	66	PHE	CD1	124.86	137.63 – 125.43	-5.5
1	A	72	GLN	CB	38.88	38.36 – 19.96	5.3
1	A	131	ASP	CB	32.21	49.06 – 32.66	-5.3
1	A	172	PRO	CG	32.94	32.66 – 21.76	5.3
1	A	179	LEU	HG	-0.22	3.16 – -0.14	-5.2
1	A	97	SER	HB3	2.44	5.25 – 2.45	-5.0

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:

