Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 02:51 PM EST

PDB ID	:	2GMO
Title	:	NMR-structure of an independently folded C-terminal domain of influenza polymerase subunit PB2
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Deposited on	:	2006-04-07

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

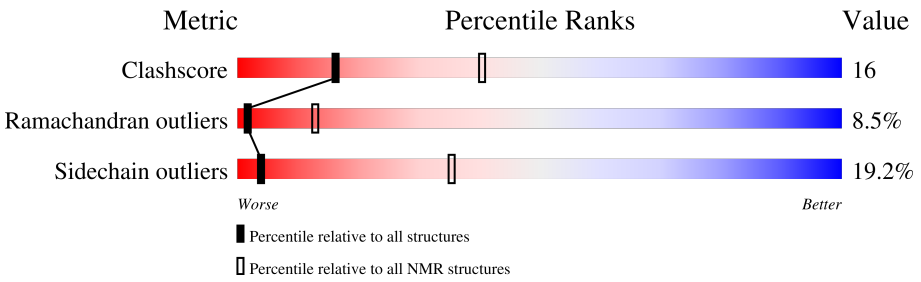
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (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	83	58% 25% 6% • 10%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 8 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:686-A:759 (74)	0.52	8

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 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 8, 10
2	3, 9
Single-model clusters	4; 5; 6; 7

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1186 atoms, of which 613 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	75	1186	355	613	108	108	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	GLY	-	cloning artifact	UNP P31345

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: Polymerase basic protein 2

Chain A: 58% 25% 6% • 10%

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: Polymerase basic protein 2

Chain A: 54% 27% 8% • 10%

4.2.2 Score per residue for model 2

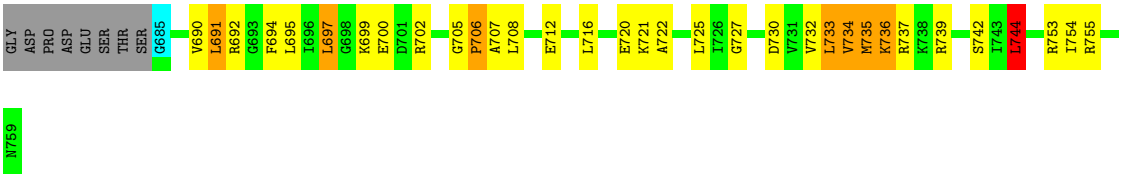
• Molecule 1: Polymerase basic protein 2

Chain A: 52% 29% 8% • 10%

4.2.3 Score per residue for model 3

- Molecule 1: Polymerase basic protein 2

Chain A: 49% 30% 8% •• 10%



4.2.4 Score per residue for model 4

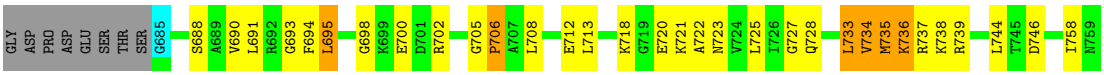
- Molecule 1: Polymerase basic protein 2

Chain A: 53% 25% 11% • 10%

4.2.5 Score per residue for model 5

- Molecule 1: Polymerase basic protein 2

Chain A: 51% 31% 7% • 10%



4.2.6 Score per residue for model 6

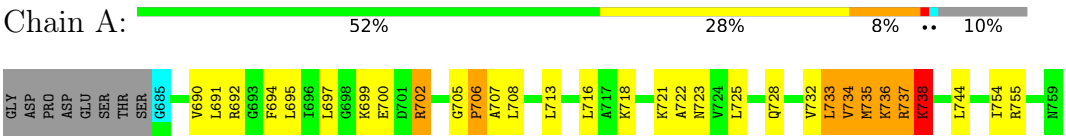
- Molecule 1: Polymerase basic protein 2

Chain A: 46% 31% 12% • 10%

4.2.7 Score per residue for model 7

- Molecule 1: Polymerase basic protein 2

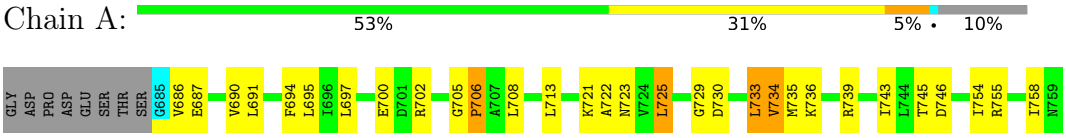
Chain A:



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Polymerase basic protein 2

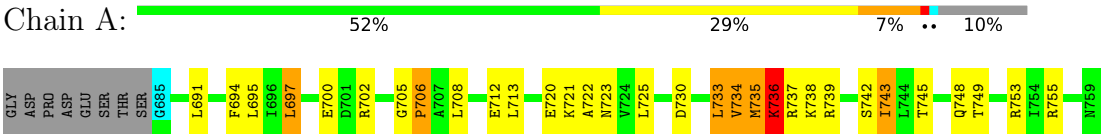
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Polymerase basic protein 2

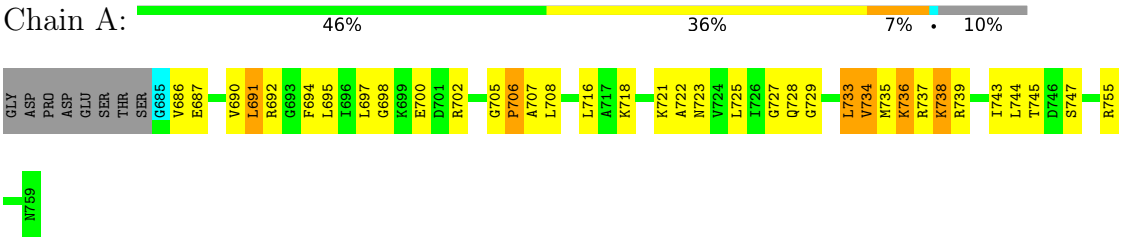
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: Polymerase basic protein 2

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *10 structures of lowest energy.*

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

Software name	Classification	Version
CNS	structure solution	cns_solve_1.1
CNS	refinement	cns_solve_1.1

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.

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	569	610	610	19±3
All	All	5690	6100	6100	187

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:733:LEU:HD23	1:A:733:LEU:H	0.66	1.50	5	3
1:A:733:LEU:H	1:A:733:LEU:HD23	0.66	1.50	9	7
1:A:700:GLU:O	1:A:733:LEU:HD21	0.64	1.91	4	1
1:A:737:ARG:HA	1:A:744:LEU:HD11	0.62	1.69	5	4
1:A:733:LEU:HD23	1:A:733:LEU:N	0.61	2.10	4	3
1:A:695:LEU:HG	1:A:744:LEU:HD22	0.61	1.71	7	1
1:A:691:LEU:HB3	1:A:694:PHE:CD1	0.58	2.33	10	9
1:A:718:LYS:HG3	1:A:738:LYS:H	0.57	1.59	5	1
1:A:725:LEU:HD13	1:A:725:LEU:H	0.55	1.60	8	1
1:A:697:LEU:HB3	1:A:754:ILE:HG23	0.55	1.78	4	1
1:A:723:ASN:N	1:A:723:ASN:HD22	0.55	1.99	4	1
1:A:722:ALA:O	1:A:733:LEU:HA	0.54	2.01	3	10
1:A:691:LEU:HD21	1:A:710:ILE:HG13	0.54	1.80	1	2
1:A:735:MET:HE2	1:A:736:LYS:O	0.54	2.02	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:743:ILE:HG13	1:A:745:THR:H	0.54	1.63	10	2
1:A:716:LEU:HD13	1:A:736:LYS:HE3	0.53	1.80	2	2
1:A:705:GLY:N	1:A:706:PRO:HD3	0.51	2.20	8	10
1:A:723:ASN:ND2	1:A:733:LEU:HD22	0.50	2.21	4	1
1:A:700:GLU:O	1:A:733:LEU:CD2	0.50	2.60	5	9
1:A:735:MET:HE2	1:A:737:ARG:N	0.50	2.21	7	2
1:A:721:LYS:HA	1:A:734:VAL:O	0.50	2.07	9	10
1:A:737:ARG:HB3	1:A:744:LEU:HD21	0.50	1.83	7	1
1:A:690:VAL:HG23	1:A:691:LEU:N	0.49	2.23	8	9
1:A:723:ASN:HA	1:A:733:LEU:HA	0.49	1.84	6	8
1:A:697:LEU:HB3	1:A:733:LEU:O	0.48	2.08	7	8
1:A:697:LEU:HD11	1:A:733:LEU:HG	0.48	1.85	4	1
1:A:715:ASN:HD22	1:A:715:ASN:N	0.47	2.06	4	1
1:A:758:ILE:HD12	1:A:758:ILE:H	0.47	1.69	5	1
1:A:716:LEU:HB2	1:A:736:LYS:HE2	0.47	1.85	1	1
1:A:736:LYS:NZ	1:A:736:LYS:HB3	0.47	2.25	1	1
1:A:695:LEU:HG	1:A:744:LEU:HD13	0.47	1.86	10	2
1:A:721:LYS:HB3	1:A:733:LEU:HD12	0.46	1.87	10	5
1:A:695:LEU:HB2	1:A:735:MET:HB3	0.46	1.87	6	1
1:A:699:LYS:HB3	1:A:732:VAL:HG12	0.46	1.88	3	3
1:A:716:LEU:HD13	1:A:736:LYS:CE	0.46	2.41	7	2
1:A:720:GLU:O	1:A:736:LYS:HG2	0.46	2.11	9	3
1:A:718:LYS:HA	1:A:736:LYS:HB2	0.46	1.88	10	3
1:A:726:ILE:HD13	1:A:726:ILE:H	0.46	1.70	6	1
1:A:741:SER:HB3	1:A:744:LEU:HA	0.46	1.88	4	1
1:A:718:LYS:HE2	1:A:737:ARG:HE	0.46	1.71	2	1
1:A:695:LEU:O	1:A:734:VAL:HG12	0.46	2.10	2	8
1:A:737:ARG:CA	1:A:744:LEU:HD11	0.46	2.40	5	1
1:A:716:LEU:HD13	1:A:736:LYS:HE2	0.45	1.89	4	2
1:A:687:GLU:O	1:A:691:LEU:HD13	0.45	2.12	10	1
1:A:725:LEU:HA	1:A:730:ASP:O	0.45	2.12	8	1
1:A:697:LEU:HA	1:A:754:ILE:N	0.44	2.26	4	1
1:A:752:LYS:N	1:A:752:LYS:HD2	0.44	2.28	6	1
1:A:738:LYS:HE3	1:A:738:LYS:HA	0.44	1.89	7	1
1:A:691:LEU:HB3	1:A:694:PHE:HD1	0.44	1.72	2	2
1:A:758:ILE:HD12	1:A:758:ILE:N	0.44	2.28	8	1
1:A:713:LEU:HD21	1:A:734:VAL:HG21	0.44	1.90	1	2
1:A:695:LEU:HD23	1:A:746:ASP:HB2	0.43	1.90	4	1
1:A:737:ARG:O	1:A:738:LYS:HB3	0.43	2.12	9	2
1:A:700:GLU:O	1:A:733:LEU:HD22	0.43	2.13	5	2
1:A:716:LEU:HD13	1:A:736:LYS:NZ	0.43	2.27	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:697:LEU:HD23	1:A:735:MET:HG3	0.43	1.91	3	1
1:A:733:LEU:N	1:A:733:LEU:CD2	0.43	2.81	4	1
1:A:695:LEU:HD23	1:A:746:ASP:HB3	0.42	1.92	1	1
1:A:756:MET:HG2	1:A:757:ALA:H	0.42	1.75	2	1
1:A:720:GLU:C	1:A:736:LYS:HZ2	0.42	2.17	5	2
1:A:702:ARG:HD3	1:A:702:ARG:H	0.42	1.73	7	1
1:A:738:LYS:HD2	1:A:738:LYS:H	0.42	1.74	10	1
1:A:710:ILE:HA	1:A:713:LEU:HB2	0.42	1.90	6	1
1:A:721:LYS:HG3	1:A:735:MET:HG2	0.42	1.92	5	1
1:A:688:SER:HB3	1:A:694:PHE:O	0.41	2.15	5	1
1:A:716:LEU:HB2	1:A:736:LYS:HE3	0.41	1.90	6	1
1:A:698:GLY:O	1:A:733:LEU:HD23	0.41	2.16	5	2
1:A:737:ARG:HG2	1:A:744:LEU:HG	0.41	1.93	3	1
1:A:702:ARG:H	1:A:702:ARG:HD3	0.41	1.75	2	1
1:A:702:ARG:HD3	1:A:702:ARG:N	0.41	2.31	7	1
1:A:746:ASP:HB2	1:A:755:ARG:HH21	0.41	1.75	8	1
1:A:713:LEU:HD13	1:A:724:VAL:HG11	0.41	1.92	6	1
1:A:695:LEU:N	1:A:735:MET:O	0.40	2.55	5	1
1:A:744:LEU:HD23	1:A:744:LEU:HA	0.40	1.83	7	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	73/83 (88%)	56±2 (76±3%)	11±2 (15±3%)	6±2 (8±3%)	2	13
All	All	730/830 (88%)	556 (76%)	112 (15%)	62 (8%)	2	13

All 24 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	706	PRO	10
1	A	739	ARG	6
1	A	693	GLY	4

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Mol	Chain	Res	Type	Models (Total)
1	A	727	GLY	4
1	A	729	GLY	4
1	A	692	ARG	4
1	A	707	ALA	4
1	A	744	LEU	3
1	A	753	ARG	3
1	A	728	GLN	3
1	A	691	LEU	2
1	A	742	SER	2
1	A	686	VAL	2
1	A	754	ILE	1
1	A	697	LEU	1
1	A	741	SER	1
1	A	746	ASP	1
1	A	716	LEU	1
1	A	737	ARG	1
1	A	738	LYS	1
1	A	736	LYS	1
1	A	743	ILE	1
1	A	749	THR	1
1	A	747	SER	1

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	62/69 (90%)	50±2 (81±4%)	12±2 (19±4%)	4 35
All	All	620/690 (90%)	501 (81%)	119 (19%)	4 35

All 26 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	702	ARG	10
1	A	708	LEU	10
1	A	725	LEU	10
1	A	733	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	734	VAL	10
1	A	735	MET	10
1	A	736	LYS	10
1	A	755	ARG	8
1	A	712	GLU	6
1	A	713	LEU	6
1	A	697	LEU	4
1	A	744	LEU	4
1	A	730	ASP	3
1	A	754	ILE	3
1	A	748	GLN	2
1	A	745	THR	2
1	A	738	LYS	2
1	A	715	ASN	1
1	A	723	ASN	1
1	A	695	LEU	1
1	A	726	ILE	1
1	A	737	ARG	1
1	A	752	LYS	1
1	A	758	ILE	1
1	A	739	ARG	1
1	A	743	ILE	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