wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2M8L
BMRB ID	:	19261
Title	:	HIV capsid dimer structure
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Deposited on	:	2013-05-23

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 (i) symbol.

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

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

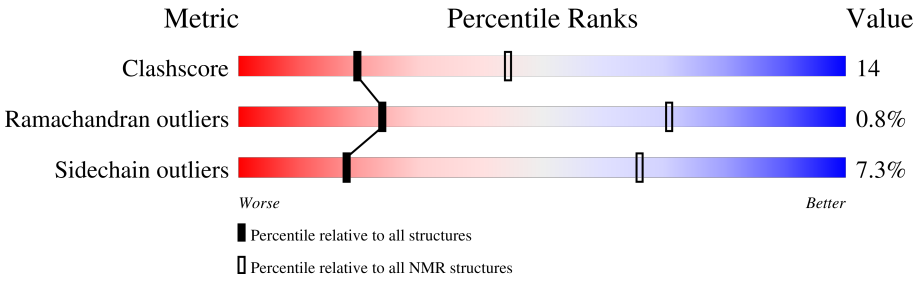
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 15%.

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	231	73% 19%
1	B	231	71% 22%

2 Ensemble composition and analysis

This entry contains 100 models. Model 95 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:1-A:145 (145)	0.05	95
2	A:150-A:221, B:150-B:221 (144)	0.06	1
3	B:1-B:145 (145)	0.06	38

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 11 clusters and 7 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 9, 10, 11, 14, 15, 16, 19, 20, 25, 26, 29, 30, 32, 33, 36, 39, 40, 41, 44, 45, 48, 53, 54, 56, 61, 64, 65, 67, 68, 71, 77, 78, 81, 84, 87, 91, 94, 95
2	7, 12, 22, 27, 42, 47, 55, 57, 62, 66, 72, 80, 86, 96
3	3, 8, 18, 28, 38, 43, 51
4	24, 31, 49, 52, 59, 74, 76
5	34, 69, 79, 83, 89
6	2, 17, 37, 82
7	23, 58, 73, 98
8	21, 60, 75, 99
9	13, 63
10	70, 85
11	50, 97
Single-model clusters	35; 46; 88; 90; 92; 93; 100

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6914 atoms, of which 3464 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein p24.

Mol	Chain	Residues	Atoms						Trace
1	A	221	Total	C	H	N	O	S	0
			3457	1088	1732	301	323	13	
1	B	221	Total	C	H	N	O	S	0
			3457	1088	1732	301	323	13	

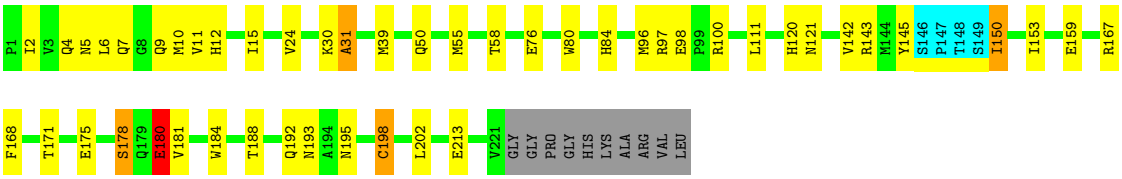
4 Residue-property plots

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.

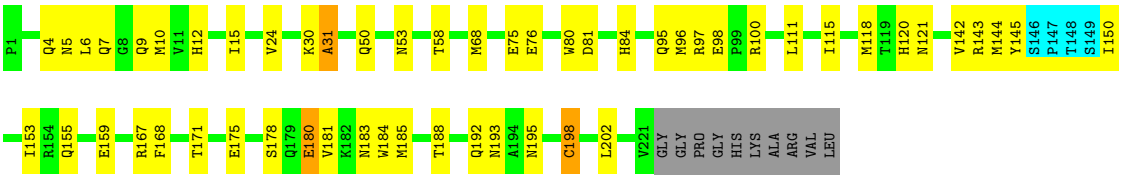
• Molecule 1: Capsid protein p24

Chain A:



• Molecule 1: Capsid protein p24

Chain B:

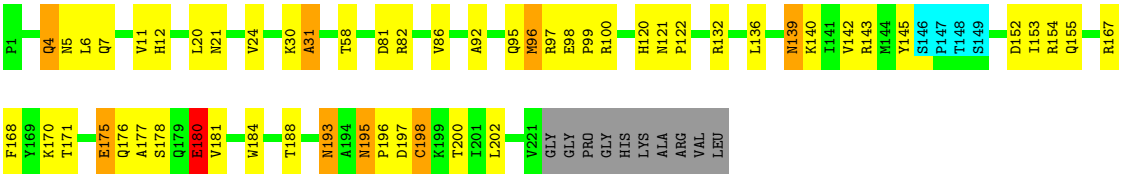


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 95. Colouring as in section 4.1 above.

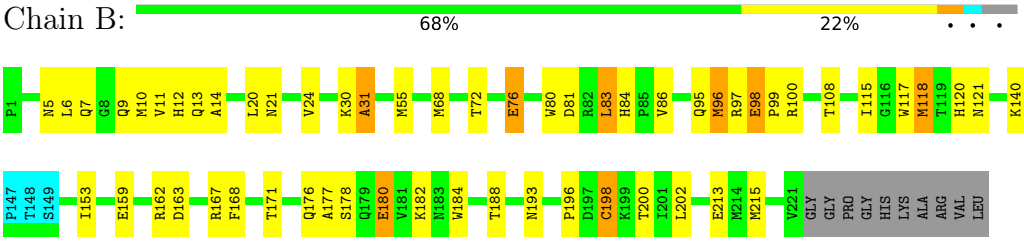
• Molecule 1: Capsid protein p24

Chain A:



• Molecule 1: Capsid protein p24

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 480 calculated structures, 100 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	refinement	2.32

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	919
Number of shifts mapped to atoms	875
Number of unparsed shifts	0
Number of shifts with mapping errors	44
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	15%

6 Model quality

6.1 Standard geometry

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	0.43±0.02	0±0/1737 (0.0± 0.0%)	0.59±0.01	1±0/2360 (0.0± 0.0%)
1	B	0.42±0.02	0±0/1737 (0.0± 0.0%)	0.57±0.01	0±1/2360 (0.0± 0.0%)
All	All	0.42	32/347400 (0.0%)	0.58	132/472000 (0.0%)

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	0.0±0.1
All	All	0	1

5 of 8 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
1	B	145	TYR	N-CA	12.10	1.70	1.46	97	7
1	A	145	TYR	CA-C	7.82	1.73	1.52	92	4
1	A	145	TYR	N-CA	7.66	1.61	1.46	84	12
1	A	145	TYR	C-N	6.32	1.48	1.34	92	1
1	B	145	TYR	CA-C	6.12	1.68	1.52	91	2

5 of 16 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	145	TYR	N-CA-CB	8.72	126.29	110.60	99	6
1	A	180	GLU	N-CA-CB	8.24	125.44	110.60	1	100
1	B	144	MET	C-N-CA	-7.73	102.37	121.70	97	4
1	B	145	TYR	N-CA-C	7.59	131.50	111.00	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	145	TYR	CA-CB-CG	-6.62	100.81	113.40	81	4

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	145	TYR	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	1699	1708	1703	51±9
1	B	1699	1708	1703	51±6
All	All	339800	341600	340600	9517

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 14.

5 of 1337 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:145:TYR:N	1:B:145:TYR:CA	1.53	1.70	97	1
1:A:179:GLN:HG3	1:A:180:GLU:OE2	1.29	1.26	59	24
1:A:179:GLN:CG	1:A:180:GLU:OE2	1.13	1.95	97	24
1:B:6:LEU:HD22	1:B:6:LEU:H	1.01	1.16	25	19
1:A:179:GLN:HG3	1:A:180:GLU:CD	0.99	1.74	97	24

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	215/231 (93%)	211±1 (98±0%)	2±1 (1±0%)	2±1 (1±0%)	24 71
1	B	215/231 (93%)	211±1 (98±0%)	2±1 (1±0%)	2±1 (1±0%)	26 73
All	All	43000/46200 (93%)	42177 (98%)	493 (1%)	330 (1%)	24 71

5 of 8 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	31	ALA	100
1	B	31	ALA	100
1	A	150	ILE	47
1	B	150	ILE	30
1	B	145	TYR	28

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	184/194 (95%)	171±3 (93±2%)	13±3 (7±2%)	19 67
1	B	184/194 (95%)	170±4 (92±2%)	14±4 (8±2%)	17 65
All	All	36800/38800 (95%)	34121 (93%)	2679 (7%)	18 66

5 of 152 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	180	GLU	100
1	B	178	SER	100
1	B	180	GLU	100
1	A	178	SER	99
1	A	198	CYS	91

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

The completeness of assignment taking into account all chemical shift lists is 15% for the well-defined parts and 15% 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

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	919
Number of shifts mapped to atoms	875
Number of unparsed shifts	0
Number of shifts with mapping errors	44
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 44) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	222	GLY	H	8.564	0.020	.
1	A	222	GLY	C	174.142	0.200	.
1	A	222	GLY	CA	44.634	0.061	.
1	A	222	GLY	N	115.571	0.200	.
1	A	223	GLY	H	7.914	0.020	.
1	A	223	GLY	C	172.071	0.200	.
1	A	223	GLY	CA	44.124	0.017	.
1	A	223	GLY	N	108.695	0.200	.
1	A	224	PRO	C	177.859	0.200	.
1	A	224	PRO	CA	63.23	0.200	.
1	A	224	PRO	CB	31.122	0.200	.
1	A	225	GLY	H	8.415	0.020	.
1	A	225	GLY	C	174.067	0.200	.
1	A	225	GLY	CA	44.876	0.046	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	225	GLY	N	109.29	0.200	.
1	A	226	HIS	H	8.049	0.020	.
1	A	226	HIS	CA	55.859	0.050	.
1	A	226	HIS	CB	28.879	0.200	.
1	A	226	HIS	N	119.896	0.001	.
1	A	227	LYS	H	8.119	0.020	.
1	A	227	LYS	C	175.898	0.200	.
1	A	227	LYS	CA	55.628	0.015	.
1	A	227	LYS	CB	31.893	0.052	.
1	A	227	LYS	N	123.533	0.001	.
1	A	228	ALA	H	8.147	0.020	.
1	A	228	ALA	C	177.383	0.200	.
1	A	228	ALA	CA	51.938	0.005	.
1	A	228	ALA	CB	18.4	0.011	.
1	A	228	ALA	N	125.611	0.200	.
1	A	229	ARG	H	8.166	0.020	.
1	A	229	ARG	C	175.894	0.200	.
1	A	229	ARG	CA	55.627	0.003	.
1	A	229	ARG	CB	29.898	0.005	.
1	A	229	ARG	N	121.107	0.200	.
1	A	230	VAL	H	8.09	0.020	.
1	A	230	VAL	C	175.019	0.200	.
1	A	230	VAL	CA	61.973	0.036	.
1	A	230	VAL	CB	31.729	0.005	.
1	A	230	VAL	N	123.017	0.200	.
1	A	231	LEU	H	7.756	0.020	.
1	A	231	LEU	C	182.069	0.200	.
1	A	231	LEU	CA	56.348	0.200	.
1	A	231	LEU	CB	42.383	0.200	.
1	A	231	LEU	N	131.803	0.200	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	200	0.09 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	173	1.36 ± 0.07	Should be checked
$^{13}C'$	190	-0.38 ± 0.11	None needed (< 0.5 ppm)
^{15}N	178	0.07 ± 0.27	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 15%, i.e. 875 atoms were assigned a chemical shift out of a possible 5948. 0 out of 62 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	709/2136 (33%)	169/866 (20%)	371/868 (43%)	169/402 (42%)
Sidechain	166/3460 (5%)	0/2258 (0%)	166/1072 (15%)	0/130 (0%)
Aromatic	0/352 (0%)	0/172 (0%)	0/150 (0%)	0/30 (0%)
Overall	875/5948 (15%)	169/3296 (5%)	537/2090 (26%)	169/562 (30%)

7.1.4 Statistically unusual chemical shifts

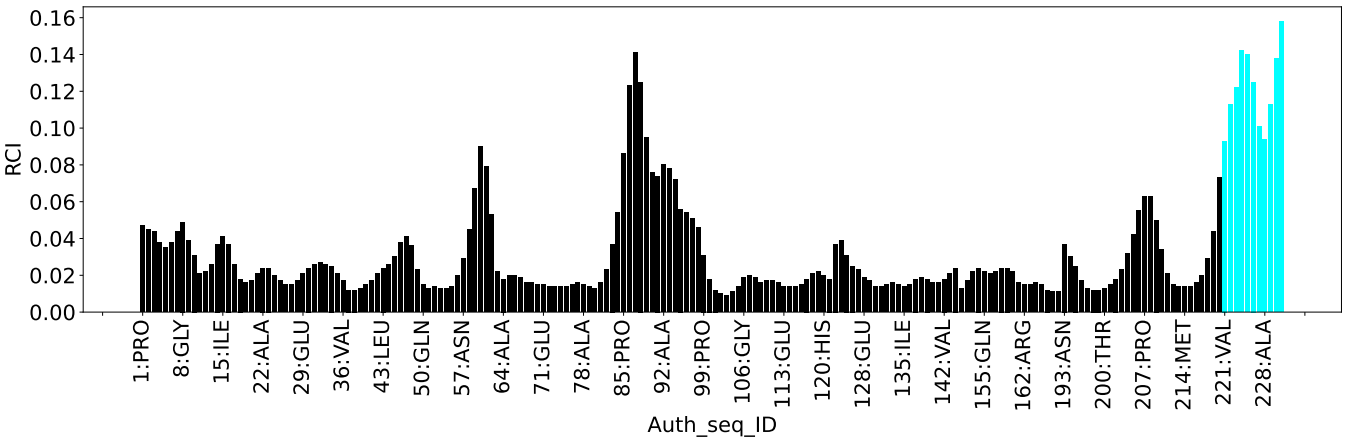
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	101	GLY	H	11.58	5.23 – 11.42	5.2

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.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:



8 NMR restraints analysis (i)

No restraints data found

9 Distance violation analysis (i)

No distance restraints data found

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found