



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KDY
Title : NMR structure of LP2086-B01
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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
<http://wwpdb.org/validation/2016/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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

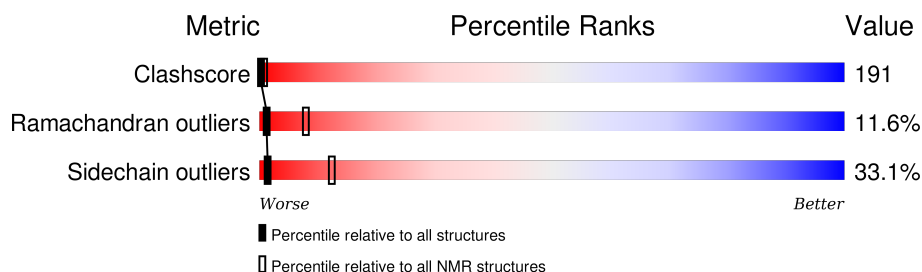
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	261	

2 Ensemble composition and analysis

This entry contains 17 models. Model 5 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:19-A:122, A:129-A:190, A:195-A:261 (233)	1.00	5

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	2, 3, 4, 5, 8, 9, 12, 14, 15, 16, 17
2	1, 7, 10, 11, 13
Single-model clusters	6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3847 atoms, of which 1900 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Factor H binding protein variant B01_001.

Mol	Chain	Residues	Atoms						Trace
1	A	261	Total	C	H	N	O	S	0
			3847	1203	1900	340	401	3	

There are 2 discrepancies between the modelled and reference sequences:

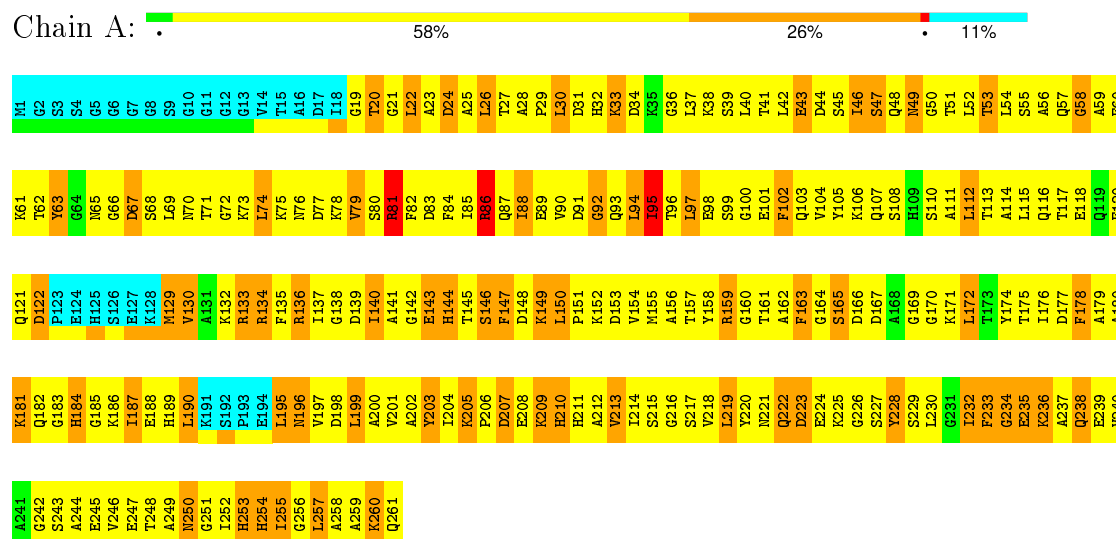
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q6VRY4
A	2	GLY	-	EXPRESSION TAG	UNP Q6VRY4

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

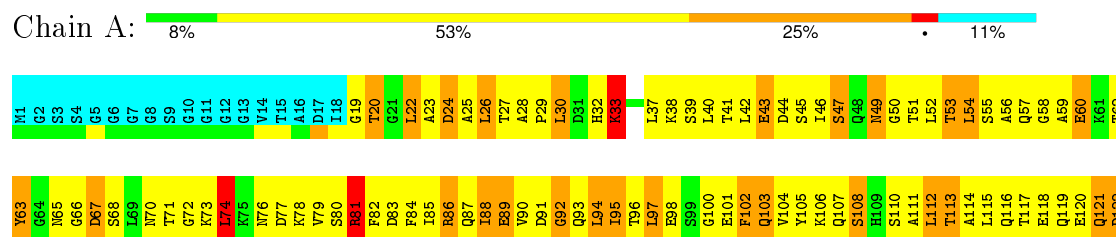
- Molecule 1: Factor H binding protein variant B01_001



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

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Factor H binding protein variant B01_001



A244	E245	V246	E247	T248	A249	V250	G251	I252	H253	H254	I255	G256	L257	A258	A259	K260	Q261																																										
H184	G185	K186	I187	E188	H189	L190	K191	S192	P193	E194	L195	M196	V197	D198	L199	A200	V201	A202	Y203	I204	K205	P206	D207	E208	K209	H210	H211	A212	V213	I214	S215	G216	S217	V218	L219	Y220	M221	Q222	D223	E224	K225	G226	S227	Y228	S229	L230	G231	I232	F233	G234	E235	K236	A237	Q238	E239	V240	A241	G242	S243
F123	E124	H125	S126	E127	K128	H129	V130	A131	K132	R133	R134	F135	R136	I137	G138	D139	I140	A141	G142	E143	H144	T145	S146	F147	D148	K149	L150	P151	K152	D153	V154	M155	A156	T157	Y158	R159	G160	T161	A162	F163	G164	S165	D166	G169	G170	K171	L172	T173	Y174	T175	I176	D177	F178	A179	A180	K181	Q182	G183	

5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 17 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	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	1.03±0.00	0±0/1795 (0.0±0.0%)	1.25±0.00	0±0/2416 (0.0±0.0%)
All	All	1.03	0/30515 (0.0%)	1.25	6/41072 (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	6.0±0.0
All	All	0	102

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	237	ALA	N-CA-CB	-5.68	102.15	110.10	4	6

There are no chirality outliers.

5 of 6 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	A	81	ARG	Sidechain	17
1	A	86	ARG	Sidechain	17
1	A	133	ARG	Sidechain	17
1	A	159	ARG	Sidechain	17
1	A	134	ARG	Sidechain	17

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	1769	1736	1736	669±33
All	All	30073	29512	29512	11366

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 191.

5 of 5011 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:PHE:CD1	1:A:212:ALA:HB2	1.25	1.66	4	15
1:A:141:ALA:HB3	1:A:144:HIS:CD2	1.21	1.70	12	2
1:A:26:LEU:HD23	1:A:54:LEU:CD1	1.19	1.67	14	6
1:A:199:LEU:CD2	1:A:218:VAL:HG22	1.17	1.68	11	6
1:A:141:ALA:HB1	1:A:233:PHE:CD2	1.16	1.75	1	4

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	232/261 (89%)	155±5 (67±2%)	50±4 (21±2%)	27±4 (12±2%)	1	8
All	All	3944/4437 (89%)	2643 (67%)	845 (21%)	456 (12%)	1	8

5 of 77 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	58	GLY	17
1	A	95	ILE	17
1	A	178	PHE	17

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Mol	Chain	Res	Type	Models (Total)
1	A	67	ASP	15
1	A	92	GLY	15

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	185/203 (91%)	124±4 (67±2%)	61±4 (33±2%)	1	12
All	All	3145/3451 (91%)	2104 (67%)	1041 (33%)	1	12

5 of 164 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	20	THR	17
1	A	255	ILE	17
1	A	22	LEU	16
1	A	49	ASN	16
1	A	102	PHE	16

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 carbohydrates 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

No chemical shift data were provided