



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 11:20 PM BST

PDB ID : 2KLF
Title : PERE NMR structure of maltodextrin-binding protein
Authors : Madl, T.; Bermel, W.; Zangger, K.
Deposited on : 2009-07-02

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

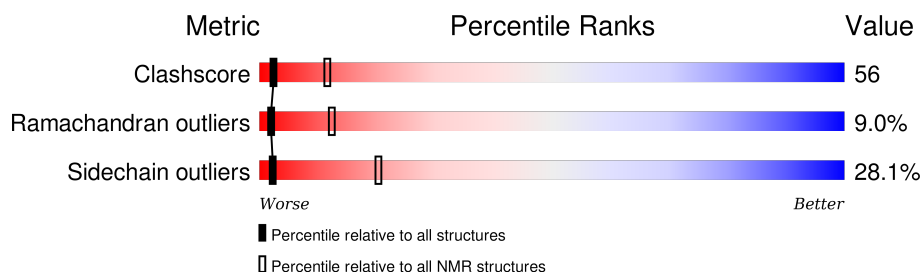
1 Overall quality at a glance

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	370	 21% 69% 9% ..

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:3-A:370 (368)	1.08	1

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 7
2	4, 8, 9
3	2, 6, 10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5735 atoms, of which 2858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms						Trace
1	A	370	Total	C	H	N	O	S	0
			5735	1851	2858	469	551	6	

There is a discrepancy between the modelled and reference sequences:

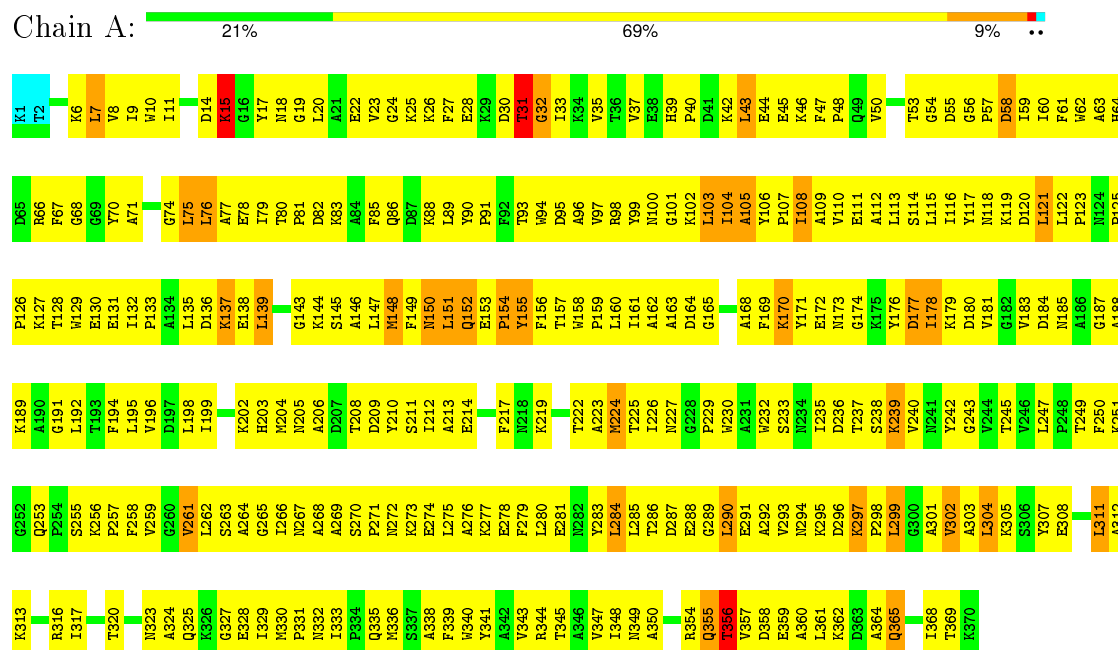
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	THR	ILE	ENGINEERED	UNP P0AEX9

4 Residue-property plots [i](#)

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.

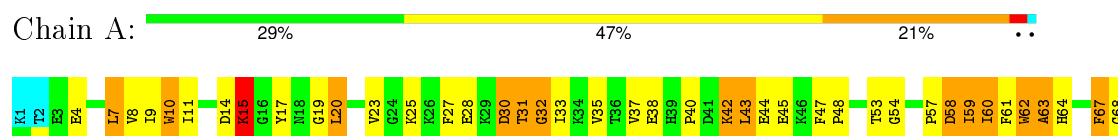
- Molecule 1: Maltose-binding periplasmic protein



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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Maltose-binding periplasmic protein



L669	A134	I199	L266	R332
Y70	L135	K200	R267	I333
A71	D136	R201	A268	P334
	K137	K202	A269	Q335
	E138	H203	S270	R336
L75	L139	H204	P271	S337
L76	K140	H205	H272	A338
A77		A206	K273	P339
E78	G143	D207	E274	
L79	K144	T208		A342
T80	S145	D209	K277	V343
P81	A146	Y210	E278	R344
D82	L147	S211	P279	T345
R83	M148	T212	L280	A346
	F149	A213		V347
	M150	E214	Y283	
L89	L151		L284	R349
Y90	Q152	F217	L285	
P91	E153	Y218	T286	R354
T92	P154	K219	D287	Q355
W94	Y155		E288	
D95	F156	T222	G289	T356
A96	T157	A223	L290	V357
V97	W158	H224	E291	D358
R98	P159	T225	A292	
Y99	L160	T226	V293	I361
N100	I161	N227	N294	R362
G101	A162	G228	K295	D363
K102	A163	P229	D296	A364
L103	D164	H230	K297	Q365
I104	G165	A231	P298	
A105		H232	L299	I368
Y106	A168		G300	T369
P107	F169	D236	A301	R370
I108	K170	T237	V302	
A109	Y171	S238	A303	
V110	E172	K239	L304	
E111	M173		K305	
A112	G174	Y242	S306	
L113	K175		Y307	
S114	Y176	T245	E308	
L115	D177	V246		
I116	I178	L247	L311	
Y117	K179		A312	
N118	D180	F250	K313	
K119	V181	K251	D314	
D120	G182	G252	P315	
L121	V183	Q253	R316	
L122		P254	I317	
P123	G187	S255		
N124	A188	K256	T320	
P125		P257	R321	
P126	G191	F258	E322	
L127	L192	V259	N323	
T128	T193	G260	A324	
H129	F194	V261	Q325	
E130	L195	L262		
E131	V196	S263	I329	
D132	D197	A264	M330	
P133	L198	G265	P331	

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing, Paramagnetic environment relaxation enhancement refinement*.

Of the 100 calculated structures, 10 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	structure solution	
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 [i](#)

6.1 Standard geometry [i](#)

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	0.33±0.01	0±0/2930 (0.0±0.0%)	0.52±0.02	1±2/3976 (0.0±0.0%)
All	All	0.33	0/29300 (0.0%)	0.52	11/39760 (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	0.7±0.5
All	All	0	7

There are no bond-length outliers.

5 of 8 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
1	A	266	ILE	CA-C-N	7.46	133.60	117.20	5	1
1	A	265	GLY	C-N-CA	7.04	139.31	121.70	5	1
1	A	266	ILE	N-CA-C	-6.94	92.25	111.00	5	1
1	A	356	THR	N-CA-C	-6.10	94.54	111.00	10	1
1	A	266	ILE	O-C-N	-5.95	113.18	122.70	5	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	354	ARG	Mainchain	7

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	2861	2836	2833	319±26
All	All	28610	28360	28330	3189

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 56.

5 of 2045 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:159:PRO:CD	1.23	1.86	7	10
1:A:170:LYS:O	1:A:176:TYR:HA	1.20	1.36	8	10
1:A:155:TYR:O	1:A:159:PRO:CG	1.19	1.89	1	10
1:A:44:GLU:O	1:A:48:PRO:CD	1.08	2.01	7	10
1:A:301:ALA:HB2	1:A:311:LEU:HD13	1.07	1.25	2	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	367/370 (99%)	281±4 (76±1%)	53±6 (15±2%)	33±5 (9±1%)	2	12
All	All	3670/3700 (99%)	2805 (76%)	534 (15%)	331 (9%)	2	12

5 of 89 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	105	ALA	10
1	A	178	ILE	10
1	A	108	ILE	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	15	LYS	10
1	A	150	ASN	10

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	295/297 (99%)	212±6 (72±2%)	83±6 (28±2%)	2	20
All	All	2950/2970 (99%)	2122 (72%)	828 (28%)	2	20

5 of 241 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	103	LEU	10
1	A	245	THR	9
1	A	7	LEU	9
1	A	139	LEU	9
1	A	170	LYS	8

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