



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KLF / pdb_00002klf
Title : PERE NMR structure of maltodextrin-binding protein
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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

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

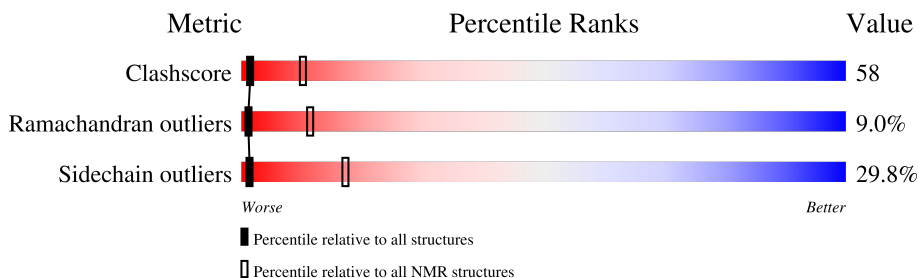
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	

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)	1.88	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

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
			Total	C	H	N	O	S	
1	A	370	5735	1851	2858	469	551	6	0

There is a discrepancy between the modelled and reference sequences:

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

G68	G69	A71	G74	L75	L76	A77	E78	I79	T80	P81	B82	K83	L89	Y90	F91	F92	T93	W94	D95	A96	W97	R98	Y99	I100	K101	K102	L103	I104	A105	Y106	P107	I108	A109	V110	E111	L112	L113	S114	L115	L116	Y117	M118	K119	D120	L121	L122	F123	M124	P125	P126	K127	L128	W129	E130	E131	I132				
P133	A134	L135	D136	K137	E138	L139	K140	G143	K144	I179	S145	A146	L147	M148	F149	M150	L151	G152	E153	P154	Y155	F156	T157	A96	W158	P159	L160	I161	M100	A162	A163	D164	G165	A168	F169	P170	K170	Y171	E172	M173	G174	A112	K175	Y176	D177	L178	K179	D180	V181	G182	V183	G187	A188	G191	L192	T193	F194	L195	V196	D197
L198	I199	K200	N201	K202	H203	M204	N205	A206	D207	T208	D209	Y210	S211	L212	A213	E214	F217	R218	K219	T222	A223	N224	T225	L226	M227	G228	P229	W230	A231	W232	A301	T237	S238	K239	Y242	T245	V246	L247	F250	K251	G252	Q253	P254	S255	K256	P257	F258	V259	G260	V261	L262	S263	A264	G265						
L266	M267	A268	A269	S270	P271	M272	K273	E274	K277	E278	F279	L280	Y283	L284	L285	T286	D287	E288	G289	L290	E291	A292	V293	M294	K295	D296	K297	P298	L299	G300	A301	V302	A303	L304	K305	S306	Y307	E308	L311	A312	K313	D314	P315	R316	I317	T320	M321	E322	N323	A324	Q325	I329	M330	P331						
N332	I333	P334	Q335	K336	S337	A338	F339	A342	V343	R344	T345	A346	V347	I348	N349	R354	Q355	T356	V357	D358	L361	K362	D363	A364	Q365	L368	T369	K370																																

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.

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	0.50±0.01	0±0/2930 (0.0± 0.0%)	0.90±0.02	10±2/3976 (0.2± 0.1%)
All	All	0.50	1/29300 (0.0%)	0.90	98/39760 (0.2%)

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

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	31	THR	N-CA	-9.19	1.40	1.46	3	1

5 of 44 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	355	GLN	N-CA-C	12.96	126.25	110.19	3	7
1	A	265	GLY	CA-C-N	9.63	139.31	121.97	5	1
1	A	265	GLY	C-N-CA	9.63	139.31	121.97	5	1
1	A	162	ALA	N-CA-C	8.93	124.15	112.72	2	1
1	A	122	LEU	CA-C-N	8.41	130.35	119.84	7	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	332±27
All	All	28610	28360	28330	3318

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 58.

5 of 2109 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%)	280±4 (76±1%)	53±6 (15±2%)	33±5 (9±1%)	1	11
All	All	3670/3700 (99%)	2805 (76%)	534 (15%)	331 (9%)	1	11

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	15	LYS	10
1	A	105	ALA	10
1	A	108	ILE	10
1	A	143	GLY	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%)	207±7 (70±2%)	88±7 (30±2%)	1	17
All	All	2950/2970 (99%)	2071 (70%)	879 (30%)	1	17

5 of 242 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	6	LYS	10
1	A	7	LEU	9
1	A	103	LEU	9
1	A	137	LYS	9
1	A	219	LYS	9

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 oligosaccharides 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