



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1Y8B / pdb_00001y8b
Title : Solution NMR-Derived Global Fold of Malate Synthase G from E.coli
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Deposited on : 2004-12-10

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

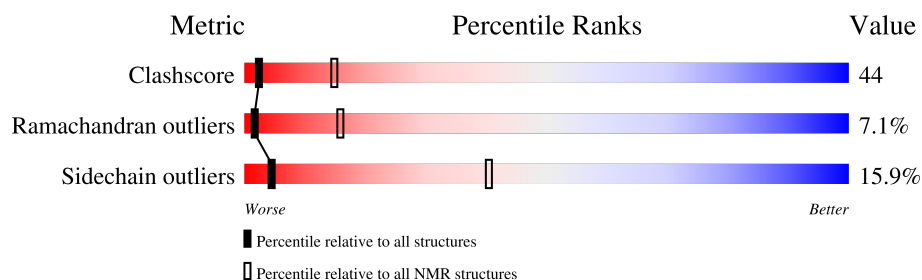
1 Overall quality at a glance

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	731	

2 Ensemble composition and analysis ⓘ

This entry contains 10 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:3-A:153, A:157-A:299, A:312-A:467, A:481-A:671, A:687-A:723 (678)	2.86	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 4 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11282 atoms, of which 5627 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Malate synthase G.

Mol	Chain	Residues	Atoms						Trace
1	A	723	Total	C	H	N	O	S	0
			11282	3543	5627	1015	1068	29	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P37330
A	2	ALA	SER	engineered mutation	UNP P37330
A	724	LEU	-	cloning artifact	UNP P37330
A	725	GLU	-	cloning artifact	UNP P37330
A	726	HIS	-	expression tag	UNP P37330
A	727	HIS	-	expression tag	UNP P37330
A	728	HIS	-	expression tag	UNP P37330
A	729	HIS	-	expression tag	UNP P37330
A	730	HIS	-	expression tag	UNP P37330
A	731	HIS	-	expression tag	UNP P37330

- Molecule 1: Malate synthase G

A676	A677	A678	P679	P680	A681	P682	P683	P684	A685	P686	P687	P688	A689	P690	P691	P692	P693	P694	P695	P696	P697	P698	P699	G700	G701	G702	G703	P704	N705	G706	G707	G708	P709	P710	P711	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165</
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5 Refinement protocol and experimental data overview

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

Of the 60 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
X-PLOR-NIH	refinement	2.9.3

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	1.47±0.00	0±0/5412 (0.0± 0.0%)	1.20±0.01	1±1/7343 (0.0± 0.0%)
All	All	1.47	3/54120 (0.0%)	1.20	10/73430 (0.0%)

All 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	A	218	GLY	N-CA	6.13	1.50	1.44	10	1
1	A	505	GLY	N-CA	5.23	1.50	1.45	4	1
1	A	136	GLY	N-CA	5.05	1.49	1.45	1	1

All 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	441	GLN	N-CA-C	-6.21	105.76	113.15	2	4
1	A	430	ARG	CB-CA-C	-6.15	109.49	116.63	6	1
1	A	8	SER	CB-CA-C	-6.14	109.50	116.63	1	3
1	A	618	SER	CB-CA-C	-5.38	109.38	115.79	3	1
1	A	448	PHE	CA-CB-CG	-5.35	108.45	113.80	9	1

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	5310	5271	5254	467±23
All	All	53100	52710	52540	4673

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 44.

5 of 3229 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:449:ILE:HD13	1:A:449:ILE:H	0.95	1.21	5	4
1:A:422:MET:O	1:A:447:ALA:HA	0.92	1.63	2	2
1:A:498:LEU:HD12	1:A:498:LEU:H	0.92	1.25	9	3
1:A:377:VAL:HG23	1:A:378:GLN:H	0.89	1.27	4	10
1:A:373:TYR:O	1:A:377:VAL:HG22	0.89	1.65	4	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	677/731 (93%)	520±10 (77±1%)	109±9 (16±1%)	48±4 (7±1%)	2	16
All	All	6770/7310 (93%)	5202 (77%)	1090 (16%)	478 (7%)	2	16

5 of 180 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	195	ASP	10
1	A	278	VAL	10
1	A	444	ASN	10
1	A	500	GLY	9
1	A	440	ALA	8

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	563/607 (93%)	473±7 (84±1%)	90±7 (16±1%)	4	40
All	All	5630/6070 (93%)	4734 (84%)	896 (16%)	4	40

5 of 375 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	498	LEU	10
1	A	105	ILE	8
1	A	335	LEU	8
1	A	449	ILE	8
1	A	10	LEU	7

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided