



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2MOI / pdb_00002moi
BMRB ID : 19943
Title : 3D NMR structure of the cytoplasmic rhodanese domain of the inner membrane protein YgaP from Escherichia coli
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Deposited on : 2014-04-26

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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

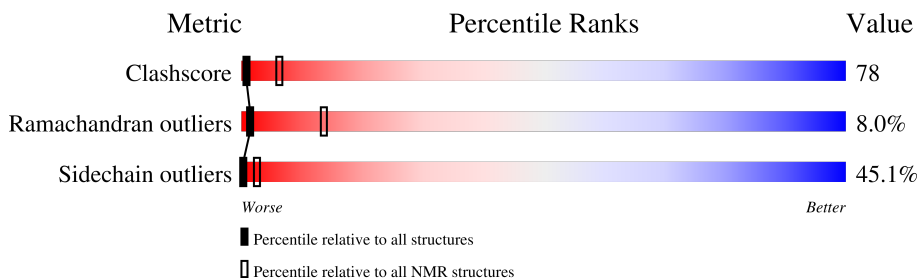
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	108	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 10 as representative, based on the following criterion: *fewest violations*.

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:63, A:69-A:104 (97)	0.69	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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 6, 10
2	4, 7, 8
Single-model clusters	9

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1528 atoms, of which 704 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Inner membrane protein YgaP.

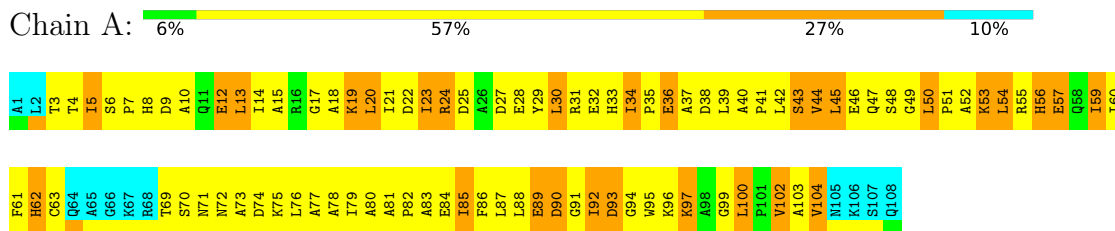
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	108	1528	519	704	147	157	1	0

4 Residue-property plots [i](#)

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.

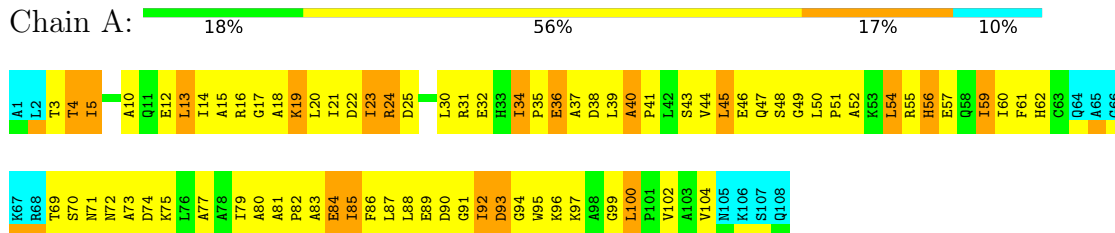
- Molecule 1: Inner membrane protein YgaP



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: Inner membrane protein YgaP



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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	1125
Number of shifts mapped to atoms	1013
Number of unparsed shifts	0
Number of shifts with mapping errors	112
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	741	635	745	116±8
All	All	7410	6350	7450	1155

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 78.

5 of 513 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:PHE:CG	1:A:76:LEU:HD12	1.05	1.86	9	1
1:A:95:TRP:CZ3	1:A:100:LEU:HD13	0.97	1.95	5	8
1:A:98:ALA:HB3	1:A:100:LEU:CD2	0.97	1.90	10	2
1:A:102:VAL:HG23	1:A:104:VAL:HG13	0.96	1.35	9	4
1:A:80:ALA:HB3	1:A:85:ILE:CD1	0.95	1.91	3	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	97/108 (90%)	61±3 (63±3%)	28±2 (29±3%)	8±2 (8±2%)	1	13
All	All	970/1080 (90%)	612 (63%)	280 (29%)	78 (8%)	1	13

5 of 29 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	30	LEU	8
1	A	89	GLU	7
1	A	56	HIS	6
1	A	39	LEU	5
1	A	83	ALA	5

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	77/85 (91%)	42±5 (55±7%)	35±5 (45±7%)	0	2
All	All	770/850 (91%)	423 (55%)	347 (45%)	0	2

5 of 61 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	14	ILE	10
1	A	19	LYS	10
1	A	23	ILE	10
1	A	24	ARG	10
1	A	34	ILE	10

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 i

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 77% 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 i

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	1125
Number of shifts mapped to atoms	1013
Number of unparsed shifts	0
Number of shifts with mapping errors	112
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	16

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 112) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	LEU	HB2	1.563	?	.
1	A	5	ILE	HG12	1.584	?	.
1	A	7	PRO	HB2	2.295	?	.
1	A	7	PRO	HD2	3.896	?	.
1	A	7	PRO	HG2	2.109	?	.
1	A	8	HIS	HB2	3.013	?	.
1	A	9	ASP	HB2	2.822	?	.
1	A	11	GLN	HB2	2.094	?	.
1	A	11	GLN	HG2	2.346	?	.
1	A	12	GLU	HB2	2.086	?	.
1	A	12	GLU	HG2	2.265	?	.
1	A	13	LEU	HB2	1.507	?	.
1	A	14	ILE	HG12	1.592	?	.
1	A	16	ARG	HB2	2.142	?	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	ARG	HD2	2.646	?	.
1	A	16	ARG	HG2	1.673	?	.
1	A	19	LYS	HB2	1.595	?	.
1	A	19	LYS	HD2	1.53	?	.
1	A	19	LYS	HE2	2.803	?	.
1	A	19	LYS	HG2	1.26	?	.
1	A	20	LEU	HB2	1.67	?	.
1	A	21	ILE	HG12	1.225	?	.
1	A	22	ASP	HB2	2.731	?	.
1	A	23	ILE	HG12	1.062	?	.
1	A	24	ARG	HB2	2.198	?	.
1	A	24	ARG	HG2	1.892	?	.
1	A	25	ASP	HB2	2.911	?	.
1	A	27	ASP	HB2	2.903	?	.
1	A	28	GLU	HB2	2.168	?	.
1	A	28	GLU	HG2	2.332	?	.
1	A	29	TYR	HB2	2.941	?	.
1	A	30	LEU	HB2	1.752	?	.
1	A	31	ARG	HB2	1.937	?	.
1	A	31	ARG	HD2	3.243	?	.
1	A	31	ARG	HG2	1.814	?	.
1	A	32	GLU	HB2	2.036	?	.
1	A	32	GLU	HG2	1.857	?	.
1	A	33	HIS	HB2	2.939	?	.
1	A	34	ILE	HG12	0.931	?	.
1	A	35	PRO	HB2	2.14	?	.
1	A	35	PRO	HD2	3.997	?	.
1	A	35	PRO	HG2	2.006	?	.
1	A	36	GLU	HB2	1.944	?	.
1	A	36	GLU	HG2	2.298	?	.
1	A	38	ASP	HB2	2.381	?	.
1	A	39	LEU	HB2	1.116	?	.
1	A	41	PRO	HB2	2.392	?	.
1	A	41	PRO	HD2	3.43	?	.
1	A	41	PRO	HG2	2.109	?	.
1	A	42	LEU	HB2	1.866	?	.
1	A	43	SER	HB2	3.877	?	.
1	A	45	LEU	HB2	1.969	?	.
1	A	46	GLU	HB2	2.009	?	.
1	A	46	GLU	HG2	2.339	?	.
1	A	47	GLN	HB2	2.159	?	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	47	GLN	HG2	2.489	?	.
1	A	48	SER	HB2	3.902	?	.
1	A	50	LEU	HB2	1.649	?	.
1	A	51	PRO	HB2	2.378	?	.
1	A	51	PRO	HG2	1.99	?	.
1	A	53	LYS	HB2	1.853	?	.
1	A	53	LYS	HD2	1.666	?	.
1	A	53	LYS	HE2	2.903	?	.
1	A	53	LYS	HG2	1.41	?	.
1	A	54	LEU	HB2	1.702	?	.
1	A	55	ARG	HB2	1.765	?	.
1	A	55	ARG	HD2	3.151	?	.
1	A	55	ARG	HG2	1.625	?	.
1	A	56	HIS	HB2	3.015	?	.
1	A	57	GLU	HB2	2.204	?	.
1	A	57	GLU	HG2	2.481	?	.
1	A	58	GLN	HB2	2.16	?	.
1	A	58	GLN	HG2	2.04	?	.
1	A	59	ILE	HG12	1.379	?	.
1	A	60	ILE	HG12	1.426	?	.
1	A	61	PHE	HB2	2.825	?	.
1	A	62	HIS	HB2	3.188	?	.
1	A	63	CYS	HB2	3.672	?	.
1	A	67	LYS	HB2	2.136	?	.
1	A	68	ARG	HD2	2.172	?	.
1	A	68	ARG	HG2	1.212	?	.
1	A	70	SER	HB2	4.001	?	.
1	A	71	ASN	HB2	2.813	?	.
1	A	72	ASN	HB2	2.637	?	.
1	A	74	ASP	HB2	2.596	?	.
1	A	75	LYS	HB2	1.806	?	.
1	A	75	LYS	HD2	1.63	?	.
1	A	75	LYS	HE2	2.932	?	.
1	A	75	LYS	HG2	1.426	?	.
1	A	76	LEU	HB2	1.526	?	.
1	A	79	ILE	HG12	1.763	?	.
1	A	82	PRO	HB2	2.46	?	.
1	A	82	PRO	HD2	3.493	?	.
1	A	82	PRO	HG2	1.899	?	.
1	A	84	GLU	HB2	2.011	?	.
1	A	84	GLU	HG2	2.204	?	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	ILE	HG12	1.45	?	.
1	A	86	PHE	HB2	2.853	?	.
1	A	87	LEU	HB2	1.895	?	.
1	A	88	LEU	HB2	2.048	?	.
1	A	89	GLU	HB2	1.946	?	.
1	A	90	ASP	HB2	2.938	?	.
1	A	92	ILE	HG12	1.187	?	.
1	A	93	ASP	HB2	3.044	?	.
1	A	95	TRP	HB2	2.884	?	.
1	A	96	LYS	HB2	1.887	?	.
1	A	97	LYS	HB2	1.941	?	.
1	A	100	LEU	HB2	0.325	?	.
1	A	101	PRO	HB2	2.287	?	.
1	A	101	PRO	HD2	3.675	?	.
1	A	101	PRO	HG2	2.125	?	.
1	A	105	ASN	HB2	2.894	?	.

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	96	0.79 ± 0.10	Should be applied
$^{13}\text{C}_\beta$	91	0.67 ± 0.17	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	100	-0.40 ± 0.38	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1051 atoms were assigned a chemical shift out of a possible 1303. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	373/478 (78%)	192/193 (99%)	90/194 (46%)	91/91 (100%)
Sidechain	646/756 (85%)	448/496 (90%)	191/238 (80%)	7/22 (32%)
Aromatic	32/69 (46%)	18/36 (50%)	12/28 (43%)	2/5 (40%)
Overall	1051/1303 (81%)	658/725 (91%)	293/460 (64%)	100/118 (85%)

7.1.4 Statistically unusual chemical shifts [i](#)

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	95	TRP	CH2	-6.33	116.19 – 131.43	-85.4
1	A	95	TRP	CZ3	-8.70	113.48 – 129.28	-82.3
1	A	95	TRP	CE3	-10.87	111.58 – 129.41	-73.7
1	A	62	HIS	CD2	26.09	103.95 – 136.66	-28.8
1	A	62	HIS	HD2	0.50	4.65 – 9.35	-13.8
1	A	24	ARG	NH2	107.99	57.68 – 87.89	11.7
1	A	24	ARG	HH11	10.68	4.72 – 9.08	8.7
1	A	34	ILE	HD11	-0.91	-0.72 – 2.09	-5.7
1	A	34	ILE	HD12	-0.91	-0.72 – 2.09	-5.7
1	A	34	ILE	HD13	-0.91	-0.72 – 2.09	-5.7
1	A	100	LEU	HD21	-0.76	-0.65 – 2.13	-5.4
1	A	100	LEU	HD22	-0.76	-0.65 – 2.13	-5.4
1	A	100	LEU	HD23	-0.76	-0.65 – 2.13	-5.4
1	A	100	LEU	HB3	-0.34	-0.26 – 3.31	-5.2
1	A	39	LEU	HB3	-0.33	-0.26 – 3.31	-5.2
1	A	64	GLN	NE2	120.71	103.38 – 120.35	5.2

7.1.5 Random Coil Index (RCI) plots [i](#)

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:

