wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1CKV
Title	:	STRUCTURE OF THE SOLUBLE METHANE MONOOXYGENASE REGULATORY PROTEIN B
Authors	:	Walters, K.J.; Gassner, G.T.; Lippard, S.J.; Wagner, G.
Deposited on	:	1999-04-25

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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

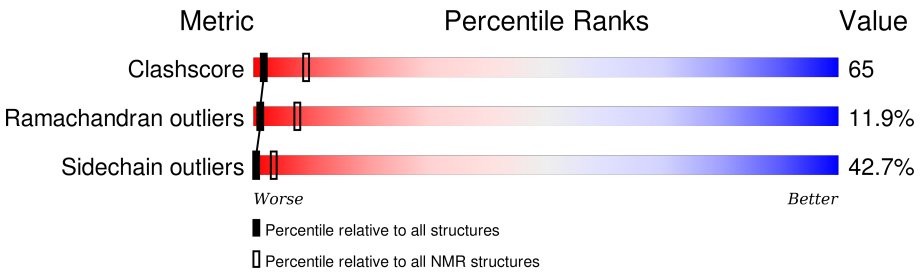
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 67%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	141	17% 39% 18% • 23%

2 Ensemble composition and analysis (i)

This entry contains 14 models. Model 2 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:9-A:23 (15)	0.98	5
2	A:36-A:128 (93)	0.36	2

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 and 1 single-model cluster was found.

Cluster number	Models
1	3, 4, 5, 11, 12, 13, 14
2	1, 2, 7, 9
3	6, 10
Single-model clusters	8

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2219 atoms, of which 1093 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (PROTEIN B).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	141	2219	713	1093	182	227	4	0

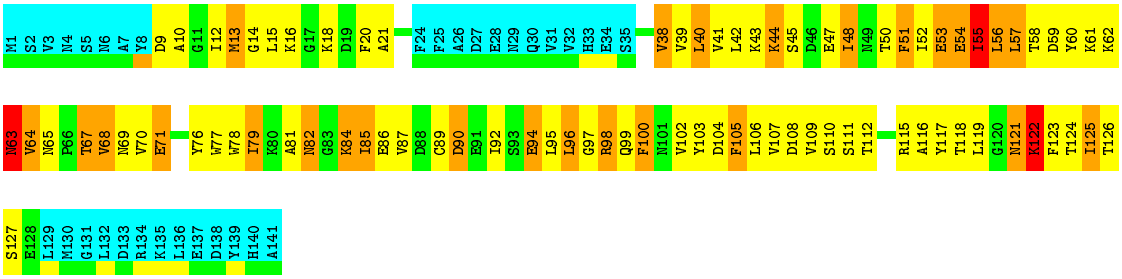
4 Residue-property plots (i)

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: PROTEIN (PROTEIN B)

Chain A: 17% 39% 18% • 23%

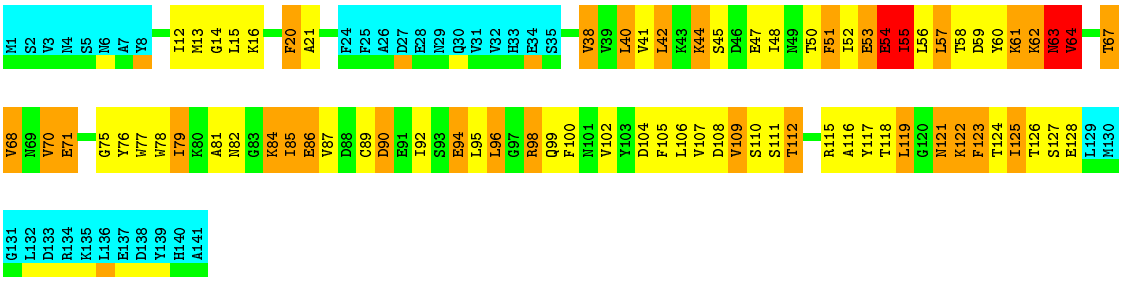


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: PROTEIN (PROTEIN B)

Chain A: 22% 31% 21% • 23%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 20 calculated structures, 14 were deposited, based on the following criterion: *NO NOE VIOLOTION GREATER THAN 0.5 ANGSTROMS AND NO DIHEDRAL ANGLE VIOLATION GREATER THAN 5 DEGREES.*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
FELIX	structure solution	
EASY	structure solution	
TALOS	structure solution	
XPLOR	structure solution	

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)	BMRB entry 4431
Number of chemical shift lists	1
Total number of shifts	1186
Number of shifts mapped to atoms	1186
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

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)

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	857	846	846	111±8
All	All	11998	11844	11844	1556

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 65.

5 of 466 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LEU:HD23	1:A:48:ILE:HD11	1.08	1.21	4	7
1:A:102:VAL:HG23	1:A:123:PHE:CD1	0.92	1.99	1	11
1:A:60:TYR:CG	1:A:68:VAL:HG11	0.91	2.00	3	9
1:A:48:ILE:HG21	1:A:77:TRP:CD1	0.91	2.01	10	14
1:A:60:TYR:CD2	1:A:68:VAL:HG11	0.89	2.03	12	7

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	108/141 (77%)	72±2 (67±2%)	23±3 (21±2%)	13±2 (12±2%)	1 7
All	All	1512/1974 (77%)	1009 (67%)	323 (21%)	180 (12%)	1 7

5 of 31 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	122	LYS	14
1	A	90	ASP	14
1	A	108	ASP	13
1	A	63	ASN	13
1	A	68	VAL	13

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	95/124 (77%)	54±3 (57±4%)	41±3 (43±4%)	0 3
All	All	1330/1736 (77%)	762 (57%)	568 (43%)	0 3

5 of 79 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	125	ILE	14
1	A	105	PHE	14
1	A	13	MET	14
1	A	82	ASN	14
1	A	38	VAL	14

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 (i)

The completeness of assignment taking into account all chemical shift lists is 67% for the well-defined parts and 64% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4431

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	1186
Number of shifts mapped to atoms	1186
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	77

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	99	7.74 ± 0.18	Should be applied
$^{13}C_{\beta}$	62	7.38 ± 0.25	Should be applied
$^{13}C'$	0	—	—
^{15}N	134	0.24 ± 0.31	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 67%, i.e. 877 atoms were assigned a chemical shift out of a possible 1311. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	398/538 (74%)	213/215 (99%)	79/216 (37%)	106/107 (99%)
Sidechain	454/672 (68%)	321/385 (83%)	121/260 (47%)	12/27 (44%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	25/101 (25%)	23/53 (43%)	0/46 (0%)	2/2 (100%)
Overall	877/1311 (67%)	557/653 (85%)	200/522 (38%)	120/136 (88%)

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.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	98	ARG	NE	113.90	92.63 – 76.73	18.4
1	A	134	ARG	NE	113.20	92.63 – 76.73	17.9
1	A	115	ARG	NE	112.30	92.63 – 76.73	17.4
1	A	73	ARG	NE	111.40	92.63 – 76.73	16.8
1	A	92	ILE	CG1	9.80	36.54 – 18.94	-10.2
1	A	18	LYS	CE	34.20	46.00 – 37.80	-9.4
1	A	73	ARG	CD	35.20	47.57 – 38.77	-9.1
1	A	134	ARG	CD	35.50	47.57 – 38.77	-8.7
1	A	98	ARG	CD	35.80	47.57 – 38.77	-8.4
1	A	128	GLU	CG	26.10	42.24 – 29.94	-8.1
1	A	95	LEU	CD1	11.70	32.77 – 16.57	-8.0
1	A	114	GLY	CA	35.50	51.81 – 38.91	-7.6
1	A	126	THR	CG2	13.20	27.15 – 15.95	-7.5
1	A	104	ASP	CA	39.80	64.88 – 44.48	-7.3
1	A	98	ARG	CG	18.50	33.23 – 21.23	-7.3
1	A	92	ILE	CG2	7.30	24.63 – 10.43	-7.2
1	A	87	VAL	CG1	11.60	28.40 – 14.60	-7.2
1	A	52	ILE	CG1	15.40	36.54 – 18.94	-7.0
1	A	23	GLN	CG	26.10	39.38 – 28.18	-6.9
1	A	99	GLN	CG	26.10	39.38 – 28.18	-6.9
1	A	42	LEU	CD2	12.50	32.60 – 15.60	-6.8
1	A	73	ARG	CG	19.10	33.23 – 21.23	-6.8
1	A	124	THR	CG2	14.10	27.15 – 15.95	-6.7
1	A	18	LYS	CG	17.30	30.67 – 19.17	-6.6
1	A	67	THR	CG2	14.20	27.15 – 15.95	-6.6
1	A	134	ARG	CG	19.50	33.23 – 21.23	-6.4
1	A	18	LYS	CD	21.40	34.86 – 23.06	-6.4
1	A	80	LYS	CG	17.60	30.67 – 19.17	-6.4
1	A	52	ILE	CG2	8.50	24.63 – 10.43	-6.4
1	A	94	GLU	CG	28.30	42.24 – 29.94	-6.3
1	A	87	VAL	CG2	11.30	29.20 – 13.40	-6.3
1	A	58	THR	CG2	14.50	27.15 – 15.95	-6.3

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	37	THR	CG2	14.50	27.15 – 15.95	-6.3
1	A	41	VAL	CG1	12.90	28.40 – 14.60	-6.2
1	A	97	GLY	CA	37.40	51.81 – 38.91	-6.2
1	A	115	ARG	CD	37.80	47.57 – 38.77	-6.1
1	A	52	ILE	CD1	3.20	21.91 – 5.01	-6.1
1	A	115	ARG	CG	20.00	33.23 – 21.23	-6.0
1	A	32	VAL	CG1	13.20	28.40 – 14.60	-6.0
1	A	75	GLY	CA	37.70	51.81 – 38.91	-5.9
1	A	118	THR	CG2	15.00	27.15 – 15.95	-5.8
1	A	28	GLU	CG	28.90	42.24 – 29.94	-5.8
1	A	53	GLU	CG	28.90	42.24 – 29.94	-5.8
1	A	34	GLU	CG	28.90	42.24 – 29.94	-5.8
1	A	71	GLU	CG	28.90	42.24 – 29.94	-5.8
1	A	40	LEU	CD2	14.20	32.60 – 15.60	-5.8
1	A	106	LEU	CD1	15.30	32.77 – 16.57	-5.8
1	A	90	ASP	CB	31.40	49.06 – 32.66	-5.8
1	A	13	MET	CG	24.80	38.33 – 25.73	-5.7
1	A	48	ILE	CD1	3.80	21.91 – 5.01	-5.7
1	A	55	ILE	CG2	9.50	24.63 – 10.43	-5.7
1	A	113	ILE	CG2	9.50	24.63 – 10.43	-5.7
1	A	96	LEU	CD2	14.50	32.60 – 15.60	-5.6
1	A	49	ASN	CB	29.20	47.13 – 30.23	-5.6
1	A	16	LYS	CB	22.90	41.68 – 23.88	-5.6
1	A	136	LEU	CD1	15.70	32.77 – 16.57	-5.5
1	A	130	MET	CG	25.10	38.33 – 25.73	-5.5
1	A	58	THR	CB	60.50	78.10 – 61.30	-5.5
1	A	121	ASN	CA	43.30	63.05 – 44.05	-5.4
1	A	107	VAL	CG1	14.20	28.40 – 14.60	-5.3
1	A	109	VAL	CB	23.20	41.76 – 23.66	-5.3
1	A	65	ASN	CA	43.60	63.05 – 44.05	-5.2
1	A	12	ILE	CG2	10.10	24.63 – 10.43	-5.2
1	A	42	LEU	CA	44.60	66.36 – 44.96	-5.2
1	A	39	VAL	CG1	14.40	28.40 – 14.60	-5.1
1	A	64	VAL	CG1	14.40	28.40 – 14.60	-5.1
1	A	81	ALA	CA	43.00	63.07 – 43.27	-5.1
1	A	107	VAL	CG2	13.20	29.20 – 13.40	-5.1
1	A	64	VAL	CG2	13.20	29.20 – 13.40	-5.1
1	A	87	VAL	HG23	-0.63	2.20 – -0.60	-5.1
1	A	87	VAL	HG22	-0.63	2.20 – -0.60	-5.1
1	A	87	VAL	HG21	-0.63	2.20 – -0.60	-5.1
1	A	74	ALA	CB	9.80	28.03 – 9.93	-5.1
1	A	117	TYR	CA	45.20	70.88 – 45.38	-5.1

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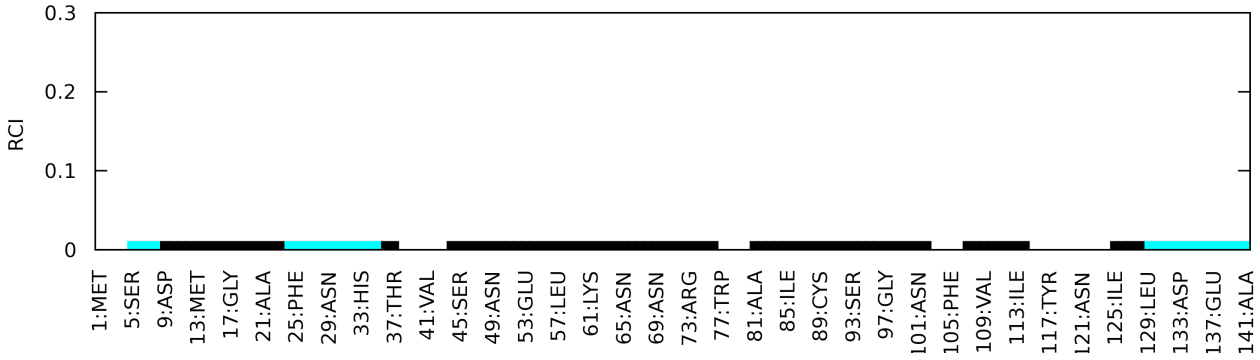
Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	71	GLU	CA	46.80	67.86 – 46.86	-5.0
1	A	86	GLU	CA	46.80	67.86 – 46.86	-5.0
1	A	39	VAL	CG2	13.40	29.20 – 13.40	-5.0

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.

Random coil index (RCI) for chain A: