



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1K1C
Title : Solution Structure of Crh, the Bacillus subtilis Catabolite Repression HPr
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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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

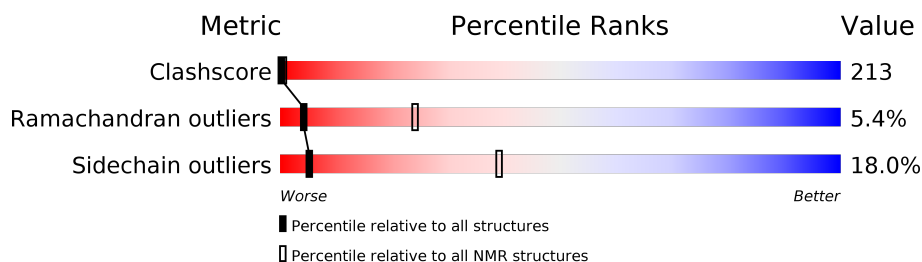
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	84	 <div style="display: flex; justify-content: space-between; width: 100%;"> . 81% 14% . </div>

2 Ensemble composition and analysis

This entry contains 24 models. Model 16 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:85 (83)	0.34	16

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 6, 7, 8, 11, 16, 17, 20, 21, 24
2	4, 13, 14, 19, 22
3	1, 3, 10
4	9, 15, 18
5	5, 12
Single-model clusters	23

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1309 atoms, of which 664 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called catabolite repression HPr-like protein.

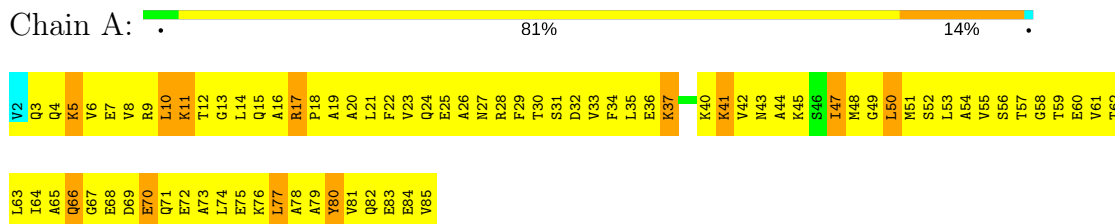
Mol	Chain	Residues	Atoms						Trace
1	A	84	Total	C	H	N	O	S	0
			1309	404	664	109	130	2	

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.

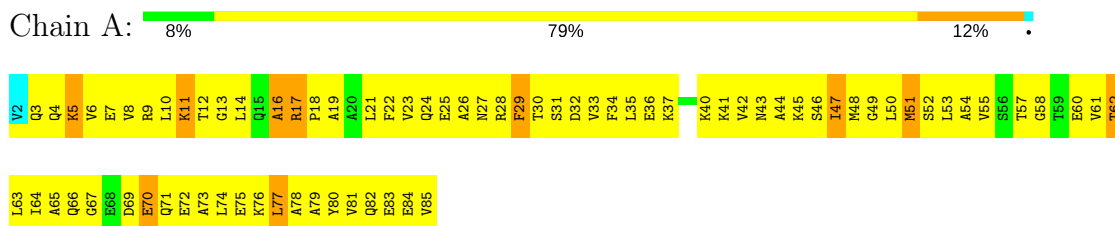
- Molecule 1: catabolite repression HPr-like protein



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

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: catabolite repression HPr-like protein



5 Refinement protocol and experimental data overview

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

Of the 250 calculated structures, 24 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
DISCOVER	structure solution	95.0
AMBER	refinement	4

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 4972, BMRB entry 5757
Number of chemical shift lists	3
Total number of shifts	1499
Number of shifts mapped to atoms	1467
Number of unparsed shifts	0
Number of shifts with mapping errors	32
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	0.53±0.01	0±0/642 (0.0±0.0%)	1.13±0.03	1±1/861 (0.1±0.1%)
All	All	0.53	0/15408 (0.0%)	1.13	24/20664 (0.1%)

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±0.2	1.0±0.6
All	All	1	24

There are no bond-length outliers.

5 of 13 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	19	ALA	N-CA-CB	-7.59	99.47	110.10	6	6
1	A	61	VAL	CA-CB-CG1	-7.03	100.36	110.90	9	3
1	A	77	LEU	CA-CB-CG	-6.84	99.56	115.30	17	1
1	A	80	TYR	CB-CG-CD2	-6.15	117.31	121.00	24	4
1	A	80	TYR	CB-CG-CD1	-5.95	117.43	121.00	6	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	59	THR	CB	1

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	80	TYR	Sidechain	15
1	A	29	PHE	Sidechain	4
1	A	22	PHE	Sidechain	3
1	A	17	ARG	Sidechain	1
1	A	9	ARG	Sidechain	1

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	638	653	653	275±14
All	All	15312	15672	15672	6595

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 213.

5 of 1641 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LYS:HB3	1:A:64:ILE:HG12	1.14	1.18	18	24
1:A:37:LYS:HA	1:A:61:VAL:HG12	1.14	1.15	11	22
1:A:31:SER:HA	1:A:67:GLY:HA3	1.14	1.19	2	24
1:A:36:GLU:HG2	1:A:41:LYS:HB2	1.12	1.16	2	24
1:A:14:LEU:HA	1:A:19:ALA:HB3	1.11	1.20	5	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	82/84 (98%)	63±3 (77±3%)	15±3 (18±3%)	4±2 (5±2%)	4	24
All	All	1968/2016 (98%)	1506 (77%)	356 (18%)	106 (5%)	4	24

5 of 22 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	70	GLU	16
1	A	37	LYS	14
1	A	17	ARG	12
1	A	16	ALA	10
1	A	10	LEU	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	68/69 (99%)	56±3 (82±4%)	12±3 (18±4%)	5	39
All	All	1632/1656 (99%)	1339 (82%)	293 (18%)	5	39

5 of 50 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	47	ILE	24
1	A	5	LYS	21
1	A	11	LYS	21
1	A	66	GLN	16
1	A	41	LYS	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

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4972

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1049
Number of shifts mapped to atoms	1017
Number of unparsed shifts	0
Number of shifts with mapping errors	32
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. First 5 (of 32) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	86	LEU	CA	54.49	0.02	1
A	86	LEU	HD11	0.79	0.1	1
A	86	LEU	HD21	0.67	0.1	1
A	87	GLN	N	121.66	0.02	1
A	86	LEU	CD2	23.12	0.02	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	85	0.30 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	79	0.56 ± 0.14	Should be applied
$^{13}\text{C}'$	82	0.48 ± 0.27	None needed (< 0.5 ppm)

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
^{15}N	83	0.02 ± 0.82	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 89%, i.e. 889 atoms were assigned a chemical shift out of a possible 1001. 10 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	407/413 (99%)	163/165 (99%)	163/166 (98%)	81/82 (99%)
Sidechain	456/553 (82%)	281/319 (88%)	168/209 (80%)	7/25 (28%)
Aromatic	26/35 (74%)	16/19 (84%)	10/16 (62%)	0/0 (—%)
Overall	889/1001 (89%)	460/503 (91%)	341/391 (87%)	88/107 (82%)

7.1.4 Statistically unusual chemical shifts [i](#)

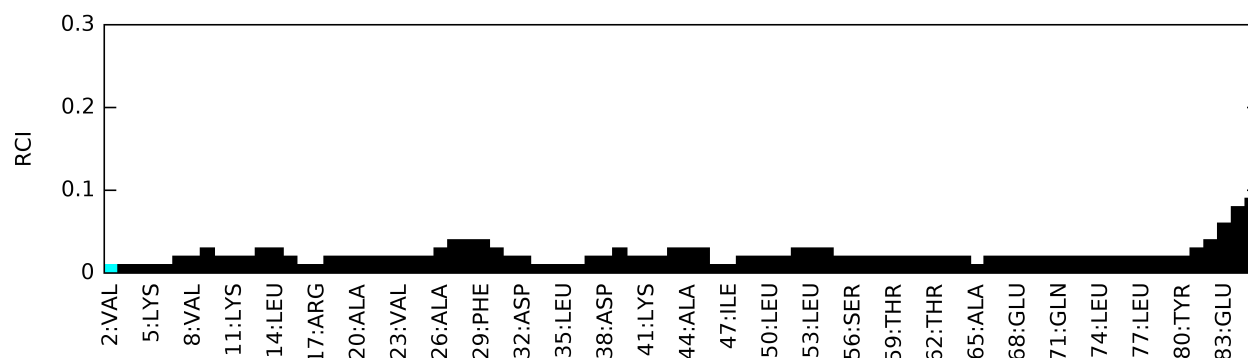
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	9	ARG	CG	36.10	33.23 – 21.23	7.4
1	A	10	LEU	CB	30.26	51.69 – 32.89	-6.4
1	A	73	ALA	HA	1.85	6.46 – 2.06	-5.5

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:



7.2 Chemical shift list 2

File name: BMRB entry 5757

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 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	440
Number of shifts mapped to atoms	440
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	84	0.26 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	79	0.09 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	57	0.37 ± 0.23	None needed (< 0.5 ppm)
^{15}N	84	0.73 ± 0.68	None needed (imprecise)

7.2.3 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 42%, i.e. 423 atoms were assigned a chemical shift out of a possible 1001. 7 out of 18 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	221/413 (54%)	0/165 (0%)	139/166 (84%)	82/82 (100%)
Sidechain	192/553 (35%)	0/319 (0%)	190/209 (91%)	2/25 (8%)
Aromatic	10/35 (29%)	0/19 (0%)	10/16 (62%)	0/0 (—%)
Overall	423/1001 (42%)	0/503 (0%)	339/391 (87%)	84/107 (79%)

7.2.4 Statistically unusual chemical shifts [i](#)

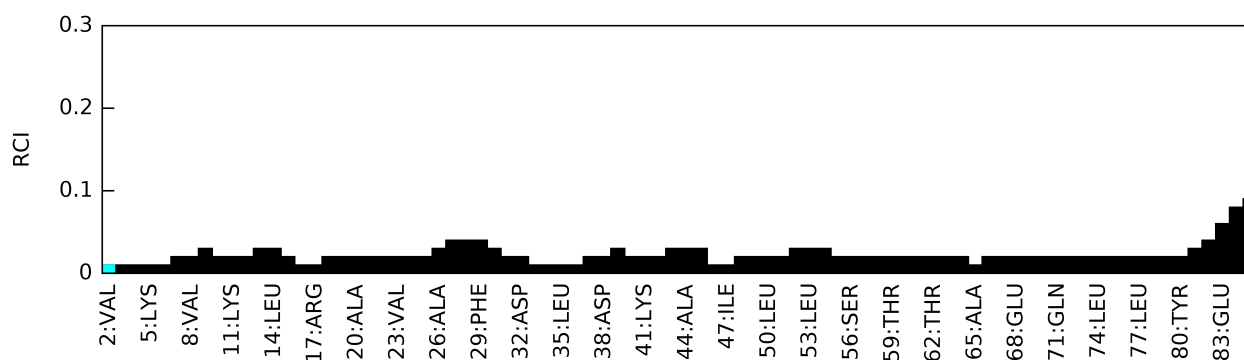
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	3	GLN	N	82.60	138.01 – 101.71	-10.3
1	A	85	VAL	N	93.40	144.09 – 98.19	-6.0

7.2.5 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:



7.3 Chemical shift list 3

File name: BMRB entry 5757

Chemical shift list name: *assigned_chem_shift_list_2*

7.3.1 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	10
Number of shifts mapped to atoms	10
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.3.3 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 1%, i.e. 10 atoms were assigned a chemical shift out of a possible 1001. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	7/413 (2%)	0/165 (0%)	3/166 (2%)	4/82 (5%)
Sidechain	3/553 (1%)	0/319 (0%)	3/209 (1%)	0/25 (0%)
Aromatic	0/35 (0%)	0/19 (0%)	0/16 (0%)	0/0 (—%)
Overall	10/1001 (1%)	0/503 (0%)	6/391 (2%)	4/107 (4%)

7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_2). RCI is only applicable to proteins.