Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:55 PM BST

PDB ID	:	1K3G
Title	:	NMR Solution Structure of Oxidized Cytochrome c-553 from Bacillus pasteurii
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Deposited on	:	2001-10-03

This is a Full wwPDB NMR Structure Validation 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:

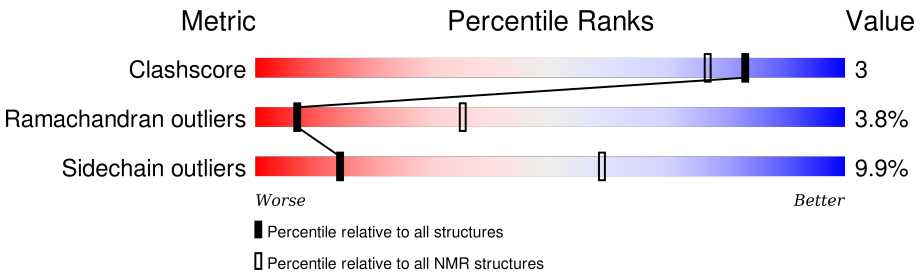
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 58%.

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	71	89% 8% ••

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 20 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:23-A:92 (70)	0.18	20

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 2 single-model clusters were found.

Cluster number	Models
1	2, 3, 5, 8, 17, 20, 24, 26, 27, 29
2	7, 9, 10, 13, 18, 19, 21, 23, 28
3	4, 6, 15, 30
4	11, 16, 25
5	1, 14
Single-model clusters	12; 22

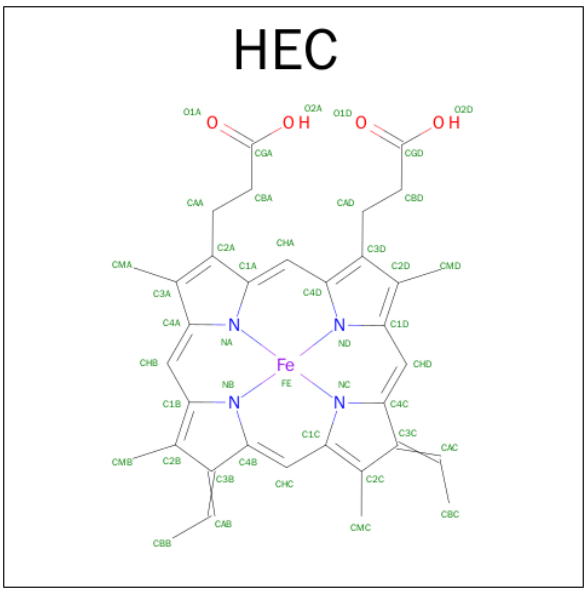
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1058 atoms, of which 518 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called cytochrome c-553.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	71	983	306	486	84	104	3	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
2	A	1	75	34	1	32	4	4

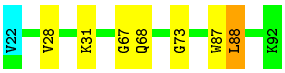
4 Residue-property plots (i)

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: cytochrome c-553

Chain A:



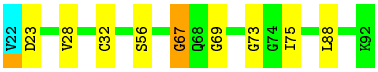
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: cytochrome c-553

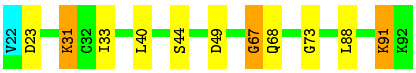
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: cytochrome c-553

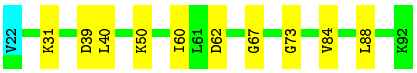
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: cytochrome c-553

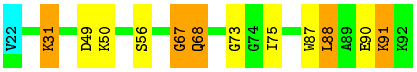
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: cytochrome c-553

Chain A:



4.2.5 Score per residue for model 5

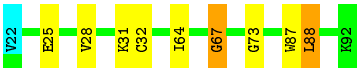
- Molecule 1: cytochrome c-553

Chain A:

4.2.6 Score per residue for model 6

- Molecule 1: cytochrome c-553

Chain A:



4.2.7 Score per residue for model 7

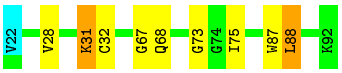
- Molecule 1: cytochrome c-553

Chain A:

4.2.8 Score per residue for model 8

- Molecule 1: cytochrome c-553

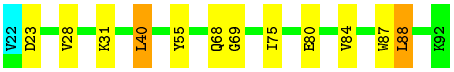
Chain A: 86% 10%



4.2.9 Score per residue for model 9

- Molecule 1: cytochrome c-553

Chain A: 82% 14%



4.2.10 Score per residue for model 10

- Molecule 1: cytochrome c-553

Chain A: 86% 11%

4.2.11 Score per residue for model 11

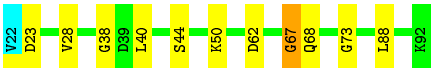
- Molecule 1: cytochrome c-553

Chain A: 79% 17%

4.2.12 Score per residue for model 12

- Molecule 1: cytochrome c-553

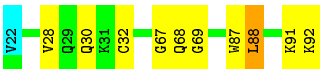
Chain A: 83% 14%



4.2.13 Score per residue for model 13

- Molecule 1: cytochrome c-553

Chain A:



4.2.14 Score per residue for model 14

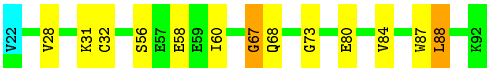
- Molecule 1: cytochrome c-553

Chain A:

4.2.15 Score per residue for model 15

- Molecule 1: cytochrome c-553

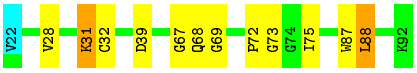
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: cytochrome c-553

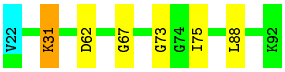
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: cytochrome c-553

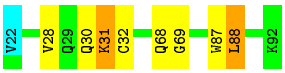
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: cytochrome c-553

Chain A: 87% 8%



4.2.19 Score per residue for model 19

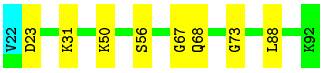
- Molecule 1: cytochrome c-553

Chain A: 76% 18%

4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: cytochrome c-553

Chain A: 87% 11%



4.2.21 Score per residue for model 21

- Molecule 1: cytochrome c-553

Chain A: 83% 14%

4.2.22 Score per residue for model 22

- Molecule 1: cytochrome c-553

Chain A: 82% 14%

4.2.23 Score per residue for model 23

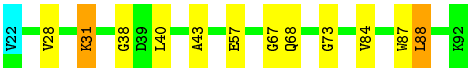
- Molecule 1: cytochrome c-553

Chain A: 87% 10%

4.2.24 Score per residue for model 24

- Molecule 1: cytochrome c-553

Chain A: 82% 14%



4.2.25 Score per residue for model 25

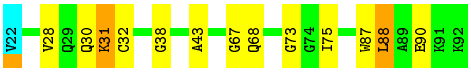
- Molecule 1: cytochrome c-553

Chain A: 87% 11%

4.2.26 Score per residue for model 26

- Molecule 1: cytochrome c-553

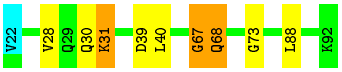
Chain A: 80% 15%



4.2.27 Score per residue for model 27

- Molecule 1: cytochrome c-553

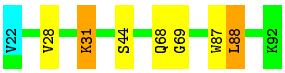
Chain A: 86% 8%



4.2.28 Score per residue for model 28

- Molecule 1: cytochrome c-553

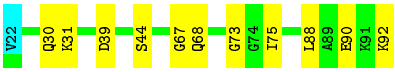
Chain A:



4.2.29 Score per residue for model 29

- Molecule 1: cytochrome c-553

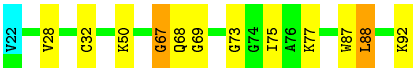
Chain A:



4.2.30 Score per residue for model 30

- Molecule 1: cytochrome c-553

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics, restrained energy minimization.*

Of the 400 calculated structures, 30 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
DYANA	structure solution	1.5
AMBER	refinement	5.0

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 5172
Number of chemical shift lists	2
Total number of shifts	550
Number of shifts mapped to atoms	518
Number of unparsed shifts	0
Number of shifts with mapping errors	32
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

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)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC

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

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	0.1±0.3
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	55	TYR	Sidechain	3

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	490	475	475	3±2
2	A	43	32	30	0±1
All	All	15990	15210	15150	94

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 3.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:VAL:HG22	1:A:32:CYS:SG	0.58	2.38	21	9
1:A:28:VAL:HG11	1:A:40:LEU:HD21	0.53	1.79	19	5
1:A:67:GLY:N	1:A:73:GLY:HA2	0.52	2.19	15	20
1:A:87:TRP:CE3	1:A:88:LEU:HD23	0.51	2.40	16	18
1:A:28:VAL:HG13	1:A:32:CYS:HB2	0.50	1.84	19	7
1:A:49:ASP:OD1	1:A:91:LYS:NZ	0.48	2.47	5	5
1:A:80:GLU:O	1:A:84:VAL:HG23	0.47	2.10	15	2
1:A:64:ILE:HD11	2:A:93:HEC:HMB2	0.45	1.88	6	4
1:A:28:VAL:HG21	1:A:87:TRP:CZ3	0.44	2.48	11	5
1:A:84:VAL:HG11	2:A:93:HEC:HMB1	0.43	1.91	9	2
1:A:28:VAL:CG1	1:A:40:LEU:HD21	0.43	2.43	9	2
1:A:87:TRP:CE3	1:A:88:LEU:CD2	0.42	3.01	4	4
1:A:60:ILE:HG23	2:A:93:HEC:HMA1	0.42	1.92	3	3
1:A:45:ALA:HB1	1:A:46:PRO:HD2	0.42	1.91	5	2
1:A:72:PRO:HD2	1:A:75:ILE:HD11	0.41	1.92	16	1
1:A:28:VAL:HG23	1:A:84:VAL:HG22	0.41	1.91	24	2
1:A:28:VAL:CG2	1:A:84:VAL:HG13	0.41	2.46	9	1
1:A:33:ILE:HG22	1:A:40:LEU:CD2	0.41	2.46	2	1
1:A:31:LYS:NZ	1:A:80:GLU:OE2	0.41	2.54	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	69/71 (97%)	59±2 (86±2%)	7±1 (10±2%)	3±1 (4±2%)	7	35
All	All	2070/2130 (97%)	1778 (86%)	214 (10%)	78 (4%)	7	35

All 7 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	68	GLN	25
1	A	31	LYS	18
1	A	67	GLY	15
1	A	69	GLY	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	38	GLY	6
1	A	43	ALA	3
1	A	72	PRO	1

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	46/47 (98%)	41±1 (90±3%)	5±1 (10±3%)	14 59
All	All	1380/1410 (98%)	1243 (90%)	137 (10%)	14 59

All 24 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	88	LEU	30
1	A	31	LYS	19
1	A	75	ILE	11
1	A	50	LYS	9
1	A	30	GLN	8
1	A	44	SER	7
1	A	23	ASP	6
1	A	56	SER	6
1	A	92	LYS	6
1	A	40	LEU	5
1	A	91	LYS	5
1	A	39	ASP	4
1	A	90	GLU	4
1	A	57	GLU	3
1	A	62	ASP	3
1	A	58	GLU	2
1	A	68	GLN	2
1	A	49	ASP	1
1	A	71	MET	1
1	A	77	LYS	1
1	A	25	GLU	1
1	A	34	SER	1

Continued on next page...

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Mol	Chain	Res	Type	Models (Total)
1	A	54	ASN	1
1	A	59	GLU	1

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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	HEC	A	93	1	24,50,50	0.82±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEC	A	93	1	19,82,82	2.22±0.07	2±0 (10±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	93	1	-	0±0,6,54,54	0±0,0,8,8

There are no bond-length outliers.

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	93	HEC	CBB-CAB-C3B	6.53	113.06	127.34	13	30
2	A	93	HEC	CBC-CAC-C3C	6.10	114.01	127.34	17	30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 58% for the well-defined parts and 57% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5172

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	518
Number of shifts mapped to atoms	518
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	38

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—
^{15}N	67	1.27 ± 0.70	None needed (imprecise)

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 58%, i.e. 426 atoms were assigned a chemical shift out of a possible 737. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	203/346 (59%)	136/138 (99%)	0/140 (0%)	67/68 (99%)
Sidechain	209/364 (57%)	204/210 (97%)	0/144 (0%)	5/10 (50%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	14/27 (52%)	13/14 (93%)	0/11 (0%)	1/2 (50%)
Overall	426/737 (58%)	353/362 (98%)	0/295 (0%)	73/80 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 57%, i.e. 430 atoms were assigned a chemical shift out of a possible 748. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	204/351 (58%)	137/140 (98%)	0/142 (0%)	67/69 (97%)
Sidechain	212/370 (57%)	207/213 (97%)	0/147 (0%)	5/10 (50%)
Aromatic	14/27 (52%)	13/14 (93%)	0/11 (0%)	1/2 (50%)
Overall	430/748 (57%)	357/367 (97%)	0/300 (0%)	73/81 (90%)

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	71	MET	HG3	-24.70	4.30 – 0.50	-71.3
1	A	36	HIS	HE1	-20.25	10.53 – 5.43	-55.4
1	A	36	HIS	HD2	26.69	9.28 – 4.78	43.7
1	A	36	HIS	HB3	15.88	5.00 – 1.10	32.9
1	A	71	MET	HB3	12.39	3.70 – 0.30	30.6
1	A	71	MET	HE3	-12.23	4.28 – -0.52	-29.4
1	A	71	MET	HE1	-12.23	4.28 – -0.52	-29.4
1	A	71	MET	HE2	-12.23	4.28 – -0.52	-29.4
1	A	63	ILE	HG21	6.23	2.13 – -0.57	20.2
1	A	63	ILE	HG22	6.23	2.13 – -0.57	20.2
1	A	63	ILE	HG23	6.23	2.13 – -0.57	20.2
1	A	36	HIS	HB2	10.16	4.91 – 1.31	19.6
1	A	36	HIS	HA	10.34	6.81 – 2.41	13.0
1	A	67	GLY	HA2	8.64	5.87 – 2.07	12.3
1	A	46	PRO	HD2	-0.53	5.45 – 1.85	-11.6
1	A	68	GLN	HB2	4.80	3.30 – 0.80	11.0
1	A	68	GLN	HB3	4.73	3.37 – 0.67	10.0
1	A	71	MET	HG2	-1.10	4.23 – 0.63	-9.8
1	A	35	CYS	HB2	6.94	5.20 – 0.70	8.9
1	A	67	GLY	HA3	6.88	5.80 – 2.00	7.8
1	A	64	ILE	HG12	-1.67	3.27 – -0.73	-7.3
1	A	36	HIS	H	13.01	11.68 – 4.78	6.9

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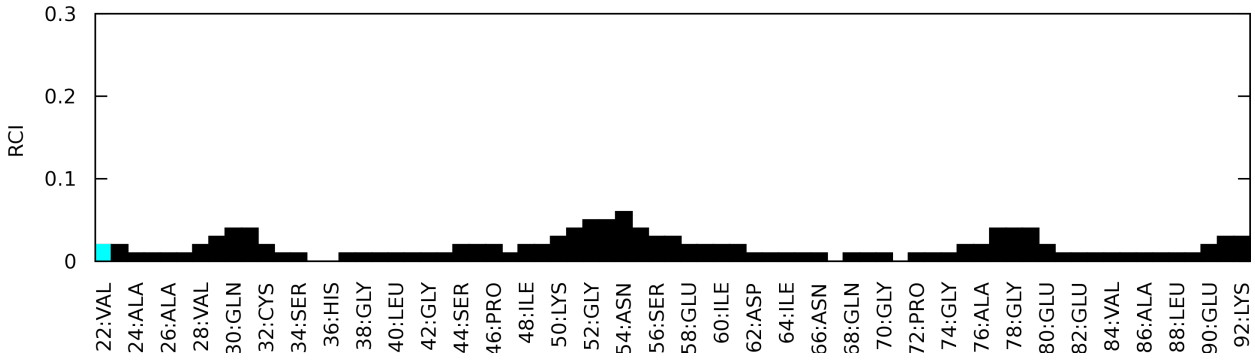
Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	71	MET	HB2	-0.30	3.73 – 0.33	-6.9
1	A	46	PRO	HG3	-0.25	3.56 – 0.26	-6.5
1	A	80	GLU	HG2	1.00	3.33 – 1.23	-6.1
1	A	48	ILE	HD11	-1.02	2.13 – -0.77	-5.9
1	A	48	ILE	HD13	-1.02	2.13 – -0.77	-5.9
1	A	48	ILE	HD12	-1.02	2.13 – -0.77	-5.9
1	A	68	GLN	H	11.57	11.17 – 5.27	5.7
1	A	71	MET	HA	1.80	6.76 – 2.06	-5.6
1	A	73	GLY	HA2	6.00	5.87 – 2.07	5.3
1	A	75	ILE	HD12	-0.86	2.13 – -0.77	-5.3
1	A	75	ILE	HD11	-0.86	2.13 – -0.77	-5.3
1	A	75	ILE	HD13	-0.86	2.13 – -0.77	-5.3
1	A	37	GLY	HA3	5.86	5.80 – 2.00	5.2
1	A	84	VAL	HG13	-0.49	2.13 – -0.47	-5.1
1	A	84	VAL	HG11	-0.49	2.13 – -0.47	-5.1
1	A	84	VAL	HG12	-0.49	2.13 – -0.47	-5.1

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 5172

Chemical shift list name: *assigned_chem_shift_list_2*

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

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

- Chain not found in structure. All 32 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEM_ox	HHB	1.46	0.02	1
UNMAPPED	1	HEM_ox	HAB	-0.21	0.02	1
UNMAPPED	1	HEM_ox	2HMC	29.18	0.02	1
UNMAPPED	1	HEM_ox	1HBC	1.78	0.02	1
UNMAPPED	1	HEM_ox	3HMC	29.18	0.02	1
UNMAPPED	1	HEM_ox	1HAA	15.72	0.02	1
UNMAPPED	1	HEM_ox	2HAD	4.32	0.02	1
UNMAPPED	1	HEM_ox	3HBC	1.78	0.02	1
UNMAPPED	1	HEM_ox	HHC	7.28	0.02	1
UNMAPPED	1	HEM_ox	HHD	-0.31	0.02	1
UNMAPPED	1	HEM_ox	2HBD	0.27	0.02	1
UNMAPPED	1	HEM_ox	1HMC	29.18	0.02	1
UNMAPPED	1	HEM_ox	3HMD	20.11	0.02	1
UNMAPPED	1	HEM_ox	2HBC	1.78	0.02	1
UNMAPPED	1	HEM_ox	1HBD	0.76	0.02	1
UNMAPPED	1	HEM_ox	2HMA	29.75	0.02	1
UNMAPPED	1	HEM_ox	3HMB	14.25	0.02	1
UNMAPPED	1	HEM_ox	2HAA	4.45	0.02	1
UNMAPPED	1	HEM_ox	HAC	0.83	0.02	1
UNMAPPED	1	HEM_ox	1HMB	14.25	0.02	1
UNMAPPED	1	HEM_ox	1HBB	-0.71	0.02	1
UNMAPPED	1	HEM_ox	2HBB	-0.71	0.02	1
UNMAPPED	1	HEM_ox	1HMA	29.75	0.02	1
UNMAPPED	1	HEM_ox	2HMB	14.25	0.02	1
UNMAPPED	1	HEM_ox	2HBA	-116.0	0.02	2
UNMAPPED	1	HEM_ox	1HMD	20.11	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEM_ox	3HMA	29.75	0.02	1
UNMAPPED	1	HEM_ox	1HAD	5.0	0.02	1
UNMAPPED	1	HEM_ox	2HMD	20.11	0.02	1
UNMAPPED	1	HEM_ox	1HBA	-1.72	0.02	2
UNMAPPED	1	HEM_ox	HHA	4.62	0.02	1
UNMAPPED	1	HEM_ox	3HBB	-0.71	0.02	1

7.2.2 Chemical shift referencing (i)

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

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 737. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/346 (0%)	0/138 (0%)	0/140 (0%)	0/68 (0%)
Sidechain	0/364 (0%)	0/210 (0%)	0/144 (0%)	0/10 (0%)
Aromatic	0/27 (0%)	0/14 (0%)	0/11 (0%)	0/2 (0%)
Overall	0/737 (0%)	0/362 (0%)	0/295 (0%)	0/80 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 748. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/351 (0%)	0/140 (0%)	0/142 (0%)	0/69 (0%)
Sidechain	0/370 (0%)	0/213 (0%)	0/147 (0%)	0/10 (0%)
Aromatic	0/27 (0%)	0/14 (0%)	0/11 (0%)	0/2 (0%)
Overall	0/748 (0%)	0/367 (0%)	0/300 (0%)	0/81 (0%)

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 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.