



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:24 PM BST

PDB ID : 1KWJ
Title : solution structure determination of the fully oxidized double mutant K9-10A cytochrome c7 from *Desulfuromonas acetoxidans*, minimized average structure
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Deposited on : 2002-01-29

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 ⓘ 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
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

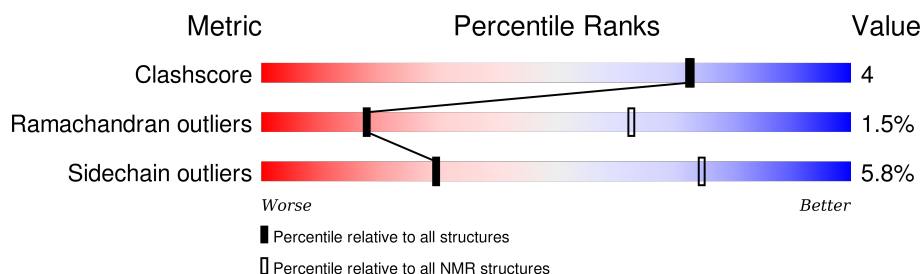
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 40%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	68	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1198 atoms, of which 572 are hydrogens and 0 are deuteriums.

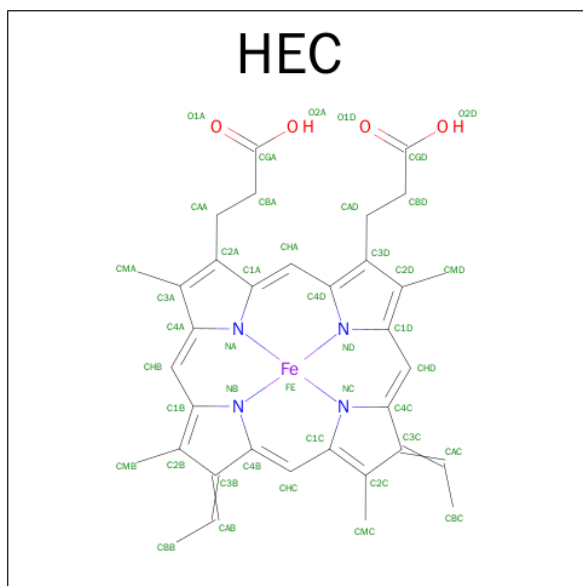
- Molecule 1 is a protein called cytochrome c7.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			973	300	476	94	97	6	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ALA	LYS	ENGINEERED	UNP P00137
A	10	ALA	LYS	ENGINEERED	UNP P00137

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

4 Residue-property plots

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 c7

Chain A:  93% 7%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing in torsion angle space; restrained energy minimization*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
PSEUDYANA	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 5279
Number of chemical shift lists	4
Total number of shifts	450
Number of shifts mapped to atoms	363
Number of unparsed shifts	0
Number of shifts with mapping errors	87
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

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	1	0
All	All	1	0

There are no bond-length outliers.

There are no bond-angle outliers.

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	1	ALA	CA

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	497	476	476	1
2	A	129	96	90	5
All	All	626	572	566	5

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:A:153:HEC:HMC1	2:A:153:HEC:HBC3	0.70	1.64
2:A:153:HEC:HMB1	2:A:153:HEC:HBB3	0.63	1.71
2:A:153:HEC:HMC1	2:A:153:HEC:CBC	0.58	2.29
2:A:153:HEC:HMD1	2:A:153:HEC:HBD1	0.53	1.81
1:A:23:LYS:NZ	2:A:153:HEC:O1D	0.48	2.47

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	66/68 (97%)	52 (79%)	13 (20%)	1 (2%)	18	63
All	All	66/68 (97%)	52 (79%)	13 (20%)	1 (2%)	18	63

All 1 Ramachandran outliers are listed below.

Mol	Chain	Res	Type
1	A	2	ASP

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	52/52 (100%)	49 (94%)	3 (6%)	29	75
All	All	52/52 (100%)	49 (94%)	3 (6%)	29	75

All 3 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	16	ASP
1	A	68	LYS

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Mol	Chain	Res	Type
1	A	43	SER

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](#)

3 ligands are 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	130	1	24,50,50	1.81	0 (0%)
2	HEC	A	153	1	24,50,50	1.71	0 (0%)
2	HEC	A	166	1	24,50,50	1.76	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	130	1	19,82,82	2.27	2 (10%)
2	HEC	A	153	1	19,82,82	1.80	1 (5%)
2	HEC	A	166	1	19,82,82	2.50	2 (10%)

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	130	1	-	0,6,54,54	0,0,8,8
2	HEC	A	153	1	-	0,6,54,54	0,0,8,8
2	HEC	A	166	1	-	0,6,54,54	0,0,8,8

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	130	HEC	CBB-CAB-C3B	6.74	112.60	127.34
2	A	166	HEC	CBB-CAB-C3B	6.49	113.16	127.34
2	A	130	HEC	CBC-CAC-C3C	6.00	114.22	127.34
2	A	166	HEC	CBC-CAC-C3C	5.95	114.33	127.34
2	A	153	HEC	CBB-CAB-C3B	5.56	115.17	127.34

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

The completeness of assignment taking into account all chemical shift lists is 40% for the well-defined parts and 40% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5279

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	363
Number of shifts mapped to atoms	363
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	80

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 40%, i.e. 301 atoms were assigned a chemical shift out of a possible 754. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	129/336 (38%)	129/134 (96%)	0/136 (0%)	0/66 (0%)
Sidechain	169/359 (47%)	169/211 (80%)	0/134 (0%)	0/14 (0%)
Aromatic	3/59 (5%)	3/33 (9%)	0/20 (0%)	0/6 (0%)
Overall	301/754 (40%)	301/378 (80%)	0/290 (0%)	0/86 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 40%, i.e. 301 atoms were assigned a chemical shift out of a possible 754. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	129/336 (38%)	129/134 (96%)	0/136 (0%)	0/66 (0%)
Sidechain	169/359 (47%)	169/211 (80%)	0/134 (0%)	0/14 (0%)
Aromatic	3/59 (5%)	3/33 (9%)	0/20 (0%)	0/6 (0%)
Overall	301/754 (40%)	301/378 (80%)	0/290 (0%)	0/86 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	53	HIS	HB2	18.13	4.91 – 1.31	41.7
1	A	45	HIS	HB3	18.60	5.00 – 1.10	39.9
1	A	45	HIS	HB2	16.22	4.91 – 1.31	36.4
1	A	53	HIS	HB3	15.55	5.00 – 1.10	32.0
1	A	30	HIS	HB3	14.33	5.00 – 1.10	28.9
1	A	17	HIS	HB2	12.64	4.91 – 1.31	26.5
1	A	17	HIS	HB3	12.88	5.00 – 1.10	25.2
1	A	66	HIS	HB3	12.38	5.00 – 1.10	23.9
1	A	20	HIS	HB2	11.55	4.91 – 1.31	23.4
1	A	30	HIS	HB2	9.88	4.91 – 1.31	18.8
1	A	66	HIS	HB2	9.71	4.91 – 1.31	18.3
1	A	44	ALA	HB2	-2.29	2.61 – 0.11	-14.6
1	A	44	ALA	HB3	-2.29	2.61 – 0.11	-14.6
1	A	44	ALA	HB1	-2.29	2.61 – 0.11	-14.6
1	A	37	ILE	HB	-2.44	3.24 – 0.34	-14.6
1	A	66	HIS	HA	10.33	6.81 – 2.41	13.0
1	A	34	PRO	HA	8.51	6.05 – 2.75	12.5
1	A	60	THR	HB	0.09	5.82 – 2.52	-12.4
1	A	13	VAL	HB	5.91	3.59 – 0.39	12.2
1	A	59	PRO	HD2	-0.70	5.45 – 1.85	-12.1
1	A	30	HIS	HA	9.73	6.81 – 2.41	11.6
1	A	50	LYS	HE3	5.12	3.86 – 1.96	11.6
1	A	2	ASP	HA	7.93	6.15 – 3.05	10.7
1	A	20	HIS	HB3	7.22	5.00 – 1.10	10.7
1	A	51	THR	HB	0.81	5.82 – 2.52	-10.2
1	A	13	VAL	HG12	3.36	2.13 – -0.47	9.7
1	A	13	VAL	HG11	3.36	2.13 – -0.47	9.7
1	A	13	VAL	HG13	3.36	2.13 – -0.47	9.7
1	A	11	GLY	HA3	7.58	5.80 – 2.00	9.7
1	A	46	LYS	HD2	3.81	2.76 – 0.46	9.6
1	A	18	LYS	HB2	4.14	3.03 – 0.53	9.4

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	34	PRO	HD2	0.26	5.45 – 1.85	-9.4
1	A	17	HIS	HA	8.71	6.81 – 2.41	9.3
1	A	37	ILE	H	1.95	11.73 – 4.83	-9.2
1	A	16	ASP	HB2	5.18	4.07 – 1.37	9.1
1	A	39	ILE	HD12	-1.93	2.13 – -0.77	-9.0
1	A	39	ILE	HD13	-1.93	2.13 – -0.77	-9.0
1	A	39	ILE	HD11	-1.93	2.13 – -0.77	-9.0
1	A	36	LYS	HA	0.32	6.46 – 2.06	-9.0
1	A	39	ILE	HG23	-1.63	2.13 – -0.57	-8.9
1	A	39	ILE	HG21	-1.63	2.13 – -0.57	-8.9
1	A	39	ILE	HG22	-1.63	2.13 – -0.57	-8.9
1	A	45	HIS	HA	8.49	6.81 – 2.41	8.8
1	A	18	LYS	HB3	4.02	3.10 – 0.40	8.4
1	A	8	ASN	HD22	11.26	9.59 – 4.69	8.4
1	A	42	LYS	HD2	3.44	2.76 – 0.46	7.9
1	A	34	PRO	HB2	4.84	3.82 – 0.32	7.9
1	A	48	ALA	HB3	-0.60	2.61 – 0.11	-7.8
1	A	48	ALA	HB1	-0.60	2.61 – 0.11	-7.8
1	A	48	ALA	HB2	-0.60	2.61 – 0.11	-7.8
1	A	36	LYS	HB2	-0.17	3.03 – 0.53	-7.8
1	A	34	PRO	HB3	4.80	3.81 – 0.21	7.7
1	A	20	HIS	HA	7.95	6.81 – 2.41	7.6
1	A	16	ASP	HA	6.88	6.15 – 3.05	7.4
1	A	18	LYS	H	12.62	11.24 – 5.14	7.3
1	A	34	PRO	HD3	0.86	5.52 – 1.72	-7.3
1	A	52	CYS	HB3	-0.49	5.25 – 0.55	-7.2
1	A	2	ASP	HB2	4.60	4.07 – 1.37	7.0
1	A	62	CYS	HB3	-0.31	5.25 – 0.55	-6.8
1	A	23	LYS	HD2	3.15	2.76 – 0.46	6.7
1	A	41	LYS	HG2	-0.31	2.67 – 0.07	-6.5
1	A	41	LYS	HA	1.44	6.46 – 2.06	-6.4
1	A	12	ASN	HA	6.88	6.52 – 2.82	6.0
1	A	16	ASP	H	11.71	11.17 – 5.47	5.9
1	A	19	ALA	HB1	2.82	2.61 – 0.11	5.8
1	A	19	ALA	HB3	2.82	2.61 – 0.11	5.8
1	A	19	ALA	HB2	2.82	2.61 – 0.11	5.8
1	A	20	HIS	H	12.17	11.68 – 4.78	5.7
1	A	37	ILE	HG23	-0.76	2.13 – -0.57	-5.7
1	A	37	ILE	HG22	-0.76	2.13 – -0.57	-5.7
1	A	37	ILE	HG21	-0.76	2.13 – -0.57	-5.7
1	A	35	ALA	H	11.59	11.19 – 5.19	5.7
1	A	67	ILE	HB	0.17	3.24 – 0.34	-5.6

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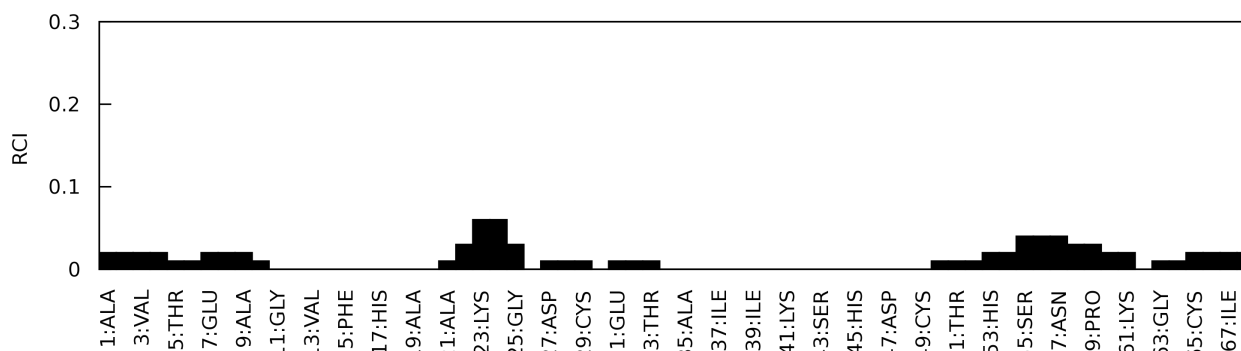
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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	61	LYS	HD2	2.86	2.76 – 0.46	5.4
1	A	62	CYS	HB2	0.51	5.20 – 0.70	-5.4
1	A	18	LYS	HA	6.64	6.46 – 2.06	5.4
1	A	62	CYS	HA	1.66	7.47 – 1.87	-5.4
1	A	2	ASP	HB3	4.14	4.07 – 1.27	5.3
1	A	26	CYS	HA	1.83	7.47 – 1.87	-5.1
1	A	30	HIS	H	11.72	11.68 – 4.78	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 5279

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	31
Number of shifts mapped to atoms	0
Number of unparsed shifts	0

Number of shifts with mapping errors	31
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 31 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HHC	0.108	-1.0	1
UNMAPPED	1	HEC	HMB1	8.629	-1.0	1
UNMAPPED	1	HEC	HMD2	9.079	-1.0	1
UNMAPPED	1	HEC	HBB1	-0.707	-1.0	1
UNMAPPED	1	HEC	HMD1	9.079	-1.0	1
UNMAPPED	1	HEC	HMA1	24.913	-1.0	1
UNMAPPED	1	HEC	HBD1	0.062	-1.0	1
UNMAPPED	1	HEC	HMA2	24.913	-1.0	1
UNMAPPED	1	HEC	HBD2	0.102	-1.0	1
UNMAPPED	1	HEC	HMC1	18.309	-1.0	1
UNMAPPED	1	HEC	HBC3	-1.855	-1.0	1
UNMAPPED	1	HEC	HAD2	1.828	-1.0	1
UNMAPPED	1	HEC	HAD1	1.124	-1.0	1
UNMAPPED	1	HEC	HMB3	8.629	-1.0	1
UNMAPPED	1	HEC	HBB2	-0.707	-1.0	1
UNMAPPED	1	HEC	HMA3	24.913	-1.0	1
UNMAPPED	1	HEC	HMC2	18.309	-1.0	1
UNMAPPED	1	HEC	HBC2	-1.855	-1.0	1
UNMAPPED	1	HEC	HAB	-1.782	-1.0	1
UNMAPPED	1	HEC	HHA	1.162	-1.0	1
UNMAPPED	1	HEC	HAA1	12.613	-1.0	1
UNMAPPED	1	HEC	HHH	4.703	-1.0	1
UNMAPPED	1	HEC	HAA2	6.903	-1.0	1
UNMAPPED	1	HEC	HMB2	8.629	-1.0	1
UNMAPPED	1	HEC	HBB3	-0.707	-1.0	1
UNMAPPED	1	HEC	HMD3	9.079	-1.0	1
UNMAPPED	1	HEC	HBA2	0.313	-1.0	1
UNMAPPED	1	HEC	HBA1	1.035	-1.0	1
UNMAPPED	1	HEC	HMC3	18.309	-1.0	1
UNMAPPED	1	HEC	HBC1	-1.855	-1.0	1
UNMAPPED	1	HEC	HAC	-2.317	-1.0	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 754. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/336 (0%)	0/134 (0%)	0/136 (0%)	0/66 (0%)
Sidechain	0/359 (0%)	0/211 (0%)	0/134 (0%)	0/14 (0%)
Aromatic	0/59 (0%)	0/33 (0%)	0/20 (0%)	0/6 (0%)
Overall	0/754 (0%)	0/378 (0%)	0/290 (0%)	0/86 (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 754. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/336 (0%)	0/134 (0%)	0/136 (0%)	0/66 (0%)
Sidechain	0/359 (0%)	0/211 (0%)	0/134 (0%)	0/14 (0%)
Aromatic	0/59 (0%)	0/33 (0%)	0/20 (0%)	0/6 (0%)
Overall	0/754 (0%)	0/378 (0%)	0/290 (0%)	0/86 (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.

7.3 Chemical shift list 3

File name: BMRB entry 5279

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	28
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	28
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 28 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HHC	-1.402	-1.0	1
UNMAPPED	1	HEC	HMB1	14.63	-1.0	1
UNMAPPED	1	HEC	HMD2	18.124	-1.0	1
UNMAPPED	1	HEC	HBB1	-1.37	-1.0	1
UNMAPPED	1	HEC	HMD1	18.124	-1.0	1
UNMAPPED	1	HEC	HMA1	-0.841	-1.0	1
UNMAPPED	1	HEC	HMA2	-0.841	-1.0	1
UNMAPPED	1	HEC	HBD2	-1.075	-1.0	1
UNMAPPED	1	HEC	HMC1	14.375	-1.0	1
UNMAPPED	1	HEC	HBC3	-0.789	-1.0	1
UNMAPPED	1	HEC	HAD1	17.774	-1.0	1
UNMAPPED	1	HEC	HMB3	14.63	-1.0	1
UNMAPPED	1	HEC	HBB2	-1.37	-1.0	1
UNMAPPED	1	HEC	HMA3	-0.841	-1.0	1
UNMAPPED	1	HEC	HMC2	14.375	-1.0	1
UNMAPPED	1	HEC	HBC2	-0.789	-1.0	1
UNMAPPED	1	HEC	HAB	-1.721	-1.0	1
UNMAPPED	1	HEC	HAA1	4.686	-1.0	1
UNMAPPED	1	HEC	HHH	10.259	-1.0	1
UNMAPPED	1	HEC	HAA2	3.105	-1.0	1
UNMAPPED	1	HEC	HMB2	14.63	-1.0	1
UNMAPPED	1	HEC	HBB3	-1.37	-1.0	1
UNMAPPED	1	HEC	HMD3	18.124	-1.0	1
UNMAPPED	1	HEC	HBA2	-1.318	-1.0	1
UNMAPPED	1	HEC	HBA1	-1.195	-1.0	1
UNMAPPED	1	HEC	HMC3	14.375	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HBC1	-0.789	-1.0	1
UNMAPPED	1	HEC	HAC	-0.778	-1.0	1

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 754. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/336 (0%)	0/134 (0%)	0/136 (0%)	0/66 (0%)
Sidechain	0/359 (0%)	0/211 (0%)	0/134 (0%)	0/14 (0%)
Aromatic	0/59 (0%)	0/33 (0%)	0/20 (0%)	0/6 (0%)
Overall	0/754 (0%)	0/378 (0%)	0/290 (0%)	0/86 (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 754. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/336 (0%)	0/134 (0%)	0/136 (0%)	0/66 (0%)
Sidechain	0/359 (0%)	0/211 (0%)	0/134 (0%)	0/14 (0%)
Aromatic	0/59 (0%)	0/33 (0%)	0/20 (0%)	0/6 (0%)
Overall	0/754 (0%)	0/378 (0%)	0/290 (0%)	0/86 (0%)

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_3). RCI is only applicable to proteins.

7.4 Chemical shift list 4

File name: BMRB entry 5279

Chemical shift list name: *assigned_chem_shift_list_4*

7.4.1 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	28
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	28
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 28 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HHC	2.048	-1.0	1
UNMAPPED	1	HEC	HMB1	15.306	-1.0	1
UNMAPPED	1	HEC	HMD2	19.556	-1.0	1
UNMAPPED	1	HEC	HBB1	2.034	-1.0	1
UNMAPPED	1	HEC	HMD1	19.556	-1.0	1
UNMAPPED	1	HEC	HMA1	12.711	-1.0	1
UNMAPPED	1	HEC	HBD1	0.141	-1.0	1
UNMAPPED	1	HEC	HMA2	12.711	-1.0	1
UNMAPPED	1	HEC	HBD2	1.156	-1.0	1
UNMAPPED	1	HEC	HMC1	9.269	-1.0	1
UNMAPPED	1	HEC	HAD2	6.075	-1.0	1
UNMAPPED	1	HEC	HAD1	4.453	-1.0	1
UNMAPPED	1	HEC	HMB3	15.306	-1.0	1
UNMAPPED	1	HEC	HBB2	2.034	-1.0	1
UNMAPPED	1	HEC	HMA3	12.711	-1.0	1
UNMAPPED	1	HEC	HMC2	9.269	-1.0	1
UNMAPPED	1	HEC	HAB	0.715	-1.0	1
UNMAPPED	1	HEC	HHA	1.158	-1.0	1
UNMAPPED	1	HEC	HAA1	1.506	-1.0	1
UNMAPPED	1	HEC	HHH	1.793	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HAA2	3.276	-1.0	1
UNMAPPED	1	HEC	HMB2	15.306	-1.0	1
UNMAPPED	1	HEC	HBB3	2.034	-1.0	1
UNMAPPED	1	HEC	HMD3	19.556	-1.0	1
UNMAPPED	1	HEC	HBA2	1.144	-1.0	1
UNMAPPED	1	HEC	HBA1	0.722	-1.0	1
UNMAPPED	1	HEC	HMC3	9.269	-1.0	1
UNMAPPED	1	HEC	HAC	0.556	-1.0	1

7.4.2 Chemical shift referencing [i](#)

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

7.4.3 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 754. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/336 (0%)	0/134 (0%)	0/136 (0%)	0/66 (0%)
Sidechain	0/359 (0%)	0/211 (0%)	0/134 (0%)	0/14 (0%)
Aromatic	0/59 (0%)	0/33 (0%)	0/20 (0%)	0/6 (0%)
Overall	0/754 (0%)	0/378 (0%)	0/290 (0%)	0/86 (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 754. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/336 (0%)	0/134 (0%)	0/136 (0%)	0/66 (0%)
Sidechain	0/359 (0%)	0/211 (0%)	0/134 (0%)	0/14 (0%)
Aromatic	0/59 (0%)	0/33 (0%)	0/20 (0%)	0/6 (0%)
Overall	0/754 (0%)	0/378 (0%)	0/290 (0%)	0/86 (0%)

7.4.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.4.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_4). RCI is only applicable to proteins.