wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1YYX
Title	:	The solution structure of a redesigned apocytochrome B562 (Rd-apocyt b562) at 2.8M urea
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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 (i) symbol.

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

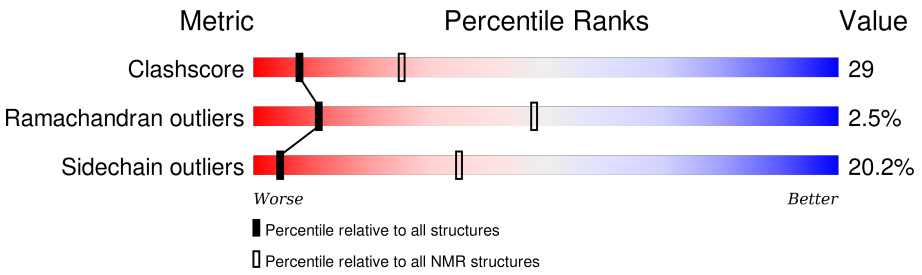
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 79%.

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	106	38% 38% 7% 18%

2 Ensemble composition and analysis (i)

This entry contains 15 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:4-A:44, A:61-A:106 (87)	0.21	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15
2	2, 14

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1641 atoms, of which 818 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Redesigned apo-cytochrome b562.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	106	1641	510	818	143	168	2	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: Redesigned apo-cytochrome b562

Chain A: 38% 38% 7% 18%

A1 D2 L3 E4 D5 N6 W7 E8 T9 L10 N11 D12 N13 L14 K15 V16 I17 E18 K19 A20 D21 N22 Q25 V26 K27 D28 M33 R34 A37 L38 D39 A40 Q41 T44 P45 P46 K47 L48 E49 D50 K51 S52 P53 D54 S55 P56 E57 M58 K59 D60 F61 R62 H63 D66

Q71 I72 D73 L76 K77 L78 A79 N80 E81 K85 Q88 A91 E92 Q93 L94 T97 Y101 N102 Q103 K104 Y105 G106

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

The representative model is number 9. Colouring as in section 4.1 above.

- Molecule 1: Redesigned apo-cytochrome b562

Chain A: 30% 39% 13% 18%

A1 D2 L3 E4 D5 N6 W7 E8 T9 L10 N11 D12 N13 L14 K15 V16 I17 E18 K19 A20 D21 N22 A23 A24 Q25 V26 K27 D28 A29 L30 M33 R34 A37 L38 D39 A40 Q41 K42 A43 T44 P45 P46 K47 L48 E49 D50 K51 S52 P53 D54 S55 P56 E57 M58 K59 D60 F61 R62

H63 D66 I67 L68 I72 D73 D74 A75 L76 K77 L78 A79 N80 E81 V84 K85 Q88 A91 E92 Q93 T97 Y101 N102 Q103 K104 Y105 G106

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry, simulated annealing, molecular dynamics, matrix relaxation, torsion angle dynamics.*

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	structure solution	NIH-2.9
X-PLOR	refinement	NIH-2.9

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 6560
Number of chemical shift lists	1
Total number of shifts	1154
Number of shifts mapped to atoms	1154
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	677	678	678	40±6
All	All	10155	10170	10170	594

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 29.

5 of 159 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HD11	1:A:94:LEU:HD13	0.95	1.39	7	5
1:A:33:MET:O	1:A:37:ALA:N	0.72	2.23	7	15
1:A:16:VAL:O	1:A:20:ALA:N	0.67	2.28	10	15
1:A:71:GLN:NE2	1:A:93:GLN:OE1	0.66	2.29	14	3
1:A:88:GLN:O	1:A:91:ALA:HB3	0.65	1.91	5	14

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	86/106 (81%)	73±1 (85±2%)	11±2 (12±2%)	2±1 (2±1%)	11 48
All	All	1290/1590 (81%)	1100 (85%)	158 (12%)	32 (2%)	11 48

All 5 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	102	ASN	14
1	A	104	LYS	13
1	A	4	GLU	2
1	A	43	ALA	2
1	A	95	LYS	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	67/85 (79%)	53±2 (80±3%)	14±2 (20±3%)	4 35
All	All	1005/1275 (79%)	802 (80%)	203 (20%)	4 35

5 of 32 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	103	GLN	15
1	A	93	GLN	15
1	A	34	ARG	15
1	A	17	ILE	15
1	A	41	GLN	15

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 79% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6560

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	1154
Number of shifts mapped to atoms	1154
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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	106	1.65 ± 0.07	Should be applied
$^{13}C_{\beta}$	102	2.37 ± 0.08	Should be applied
$^{13}C'$	0	—	—
^{15}N	98	0.40 ± 0.24	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 79%, i.e. 838 atoms were assigned a chemical shift out of a possible 1058. 12 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	346/435 (80%)	174/174 (100%)	87/174 (50%)	85/87 (98%)
Sidechain	466/570 (82%)	279/328 (85%)	175/211 (83%)	12/31 (39%)

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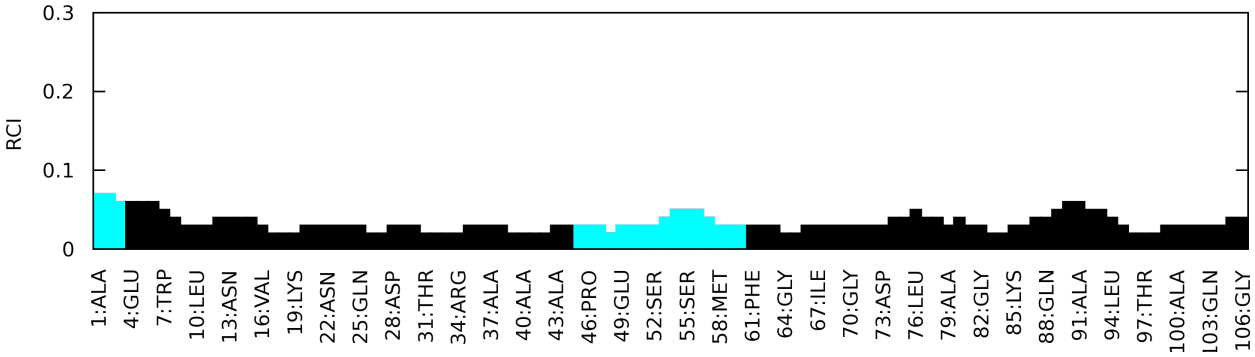
	Total	^{1}H	^{13}C	^{15}N
Aromatic	26/53 (49%)	26/28 (93%)	0/23 (0%)	0/2 (0%)
Overall	838/1058 (79%)	479/530 (90%)	262/408 (64%)	97/120 (81%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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: