wwPDB NMR Structure Validation Summary Report

Jun 12, 2024 – 03:05 PM EDT

PDB ID	:	1L6U
BMRB ID	:	4566
Title	:	NMR STRUCTURE OF OXIDIZED ADRENODOXIN
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Deposited on	:	2002-03-14

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

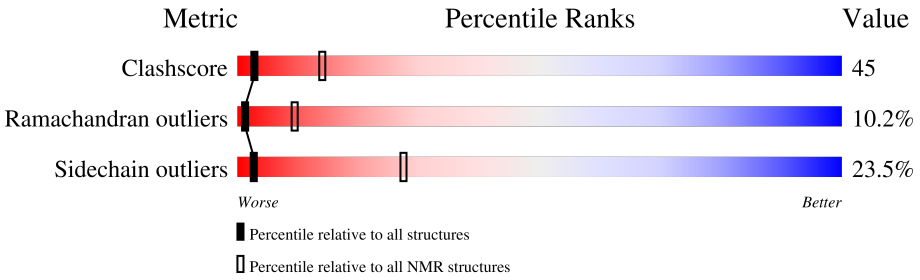
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 70%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	128	24% 44% 10% • 5% 16%

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:5-A:40, A:44-A:108 (101)	0.82	6

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 and 1 single-model cluster was found.

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

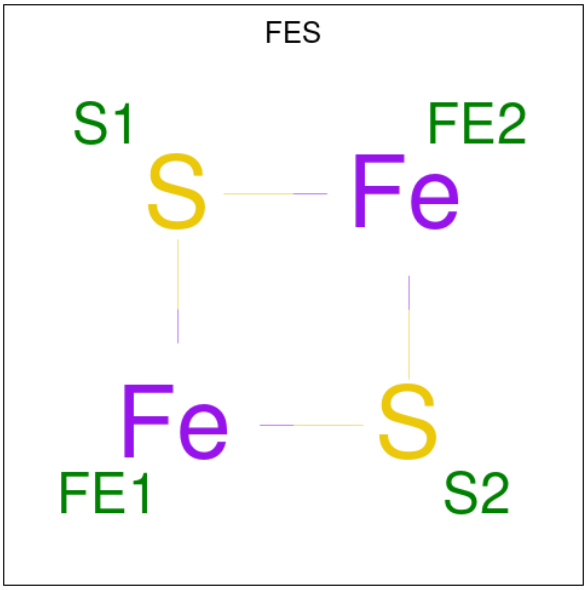
3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1652 atoms, of which 828 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adrenodoxin 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	108	1648	510	828	131	171	8	0

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



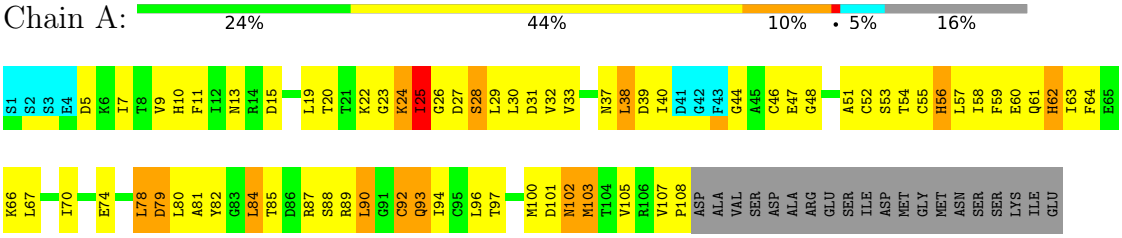
Mol	Chain	Residues	Atoms		
			Total	Fe	S
2	A	1	4	2	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

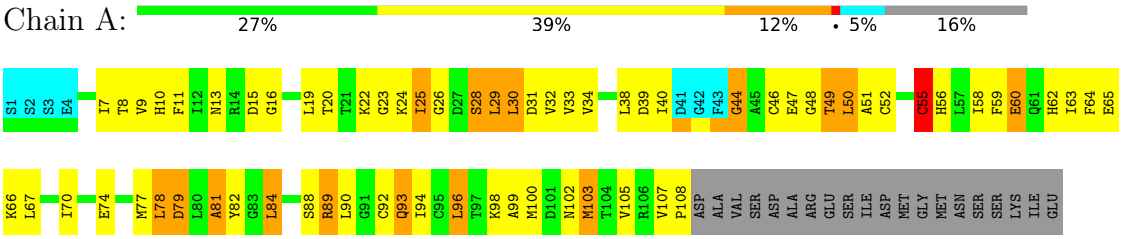
- Molecule 1: Adrenodoxin 1



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

The representative model is number 6. Colouring as in section 4.1 above.

- Molecule 1: Adrenodoxin 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, simulated annealing.*

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	1.5

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1097
Number of shifts mapped to atoms	978
Number of unparsed shifts	0
Number of shifts with mapping errors	119
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	70%

6 Model quality

6.1 Standard geometry

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

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

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	770	789	742	69±6
2	A	4	0	0	7±2
All	All	7740	7890	7419	687

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 45.

5 of 359 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:CYS:SG	2:A:146:FES:FE1	1.07	1.45	10	10
1:A:40:ILE:HG21	1:A:107:VAL:HG21	1.01	1.31	5	7
1:A:30:LEU:HD22	1:A:92:CYS:SG	0.92	2.05	3	3
1:A:38:LEU:HD13	1:A:40:ILE:HD12	0.92	1.42	3	1
1:A:52:CYS:HG	2:A:146:FES:FE1	0.88	0.67	9	10

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	100/128 (78%)	72±3 (72±3%)	18±3 (18±3%)	10±3 (10±3%)	1 9
All	All	1000/1280 (78%)	716 (72%)	182 (18%)	102 (10%)	1 9

5 of 34 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	25	ILE	10
1	A	51	ALA	10
1	A	24	LYS	6
1	A	101	ASP	5
1	A	93	GLN	5

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	84/112 (75%)	64±4 (77±5%)	20±4 (23±5%)	3 27
All	All	840/1120 (75%)	643 (77%)	197 (23%)	3 27

5 of 52 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	79	ASP	10
1	A	82	TYR	10
1	A	15	ASP	9
1	A	78	LEU	9
1	A	38	LEU	8

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 monosaccharides 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	FES	A	146	1	0,4,4	0.00±0.00	-

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	FES	A	146	1	-	-	-

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	FES	A	146	1	-	-	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

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 70% for the well-defined parts and 69% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	1097
Number of shifts mapped to atoms	978
Number of unparsed shifts	0
Number of shifts with mapping errors	119
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.

- No matching atom found in the structure. First 5 (of 119) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	ASP	H	8.47	0.022	1
1	A	109	ASP	HA	4.39	0.022	1
1	A	109	ASP	HB2	2.74	0.022	2
1	A	109	ASP	HB3	2.67	0.022	2
1	A	109	ASP	C	175.15	0.03	1
1	A	109	ASP	CA	54.34	0.03	1
1	A	109	ASP	CB	40.76	0.03	1
1	A	109	ASP	N	120.03	0.04	1
1	A	110	ALA	H	8.16	0.022	1
1	A	110	ALA	HA	4.3	0.022	1
1	A	110	ALA	HB1	1.17	0.022	1
1	A	110	ALA	HB2	1.17	0.022	1
1	A	110	ALA	HB3	1.17	0.022	1
1	A	110	ALA	C	176.75	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	110	ALA	CA	51.07	0.03	1
1	A	110	ALA	CB	19.37	0.03	1
1	A	110	ALA	N	122.28	0.04	1
1	A	111	VAL	H	7.85	0.022	1
1	A	111	VAL	HA	3.85	0.022	1
1	A	111	VAL	HB	1.82	0.022	1
1	A	111	VAL	HG11	0.78	0.022	2
1	A	111	VAL	HG12	0.78	0.022	2
1	A	111	VAL	HG13	0.78	0.022	2
1	A	111	VAL	C	174.81	0.03	1
1	A	111	VAL	CA	61.43	0.03	1
1	A	111	VAL	CB	32.11	0.03	1
1	A	111	VAL	CG1	20.06	0.03	2
1	A	111	VAL	CG2	19.8	0.03	2
1	A	111	VAL	N	118.11	0.04	1
1	A	112	SER	H	8.12	0.022	1
1	A	112	SER	HA	4.14	0.022	1
1	A	112	SER	HB2	3.83	0.022	2
1	A	112	SER	HB3	3.79	0.022	2
1	A	112	SER	C	178.24	0.03	1
1	A	112	SER	CA	57.4	0.03	1
1	A	112	SER	CB	63.24	0.03	1
1	A	112	SER	N	118.68	0.04	1
1	A	113	ASP	H	8.2	0.022	1
1	A	113	ASP	HA	4.18	0.022	1
1	A	113	ASP	HB2	2.97	0.022	2
1	A	113	ASP	HB3	2.81	0.022	2
1	A	113	ASP	C	175.73	0.03	1
1	A	113	ASP	CA	53.51	0.03	1
1	A	113	ASP	CB	40.55	0.03	1
1	A	113	ASP	N	123.19	0.04	1
1	A	114	ALA	H	8.23	0.022	1
1	A	114	ALA	HA	4.26	0.022	1
1	A	114	ALA	HB1	1.34	0.022	1
1	A	114	ALA	HB2	1.34	0.022	1
1	A	114	ALA	HB3	1.34	0.022	1
1	A	114	ALA	CA	52.0	0.03	1
1	A	114	ALA	CB	18.5	0.03	1
1	A	114	ALA	N	124.84	0.04	1
1	A	115	ARG	H	8.28	0.022	1
1	A	115	ARG	HA	4.26	0.022	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	115	ARG	HB2	1.8	0.022	2
1	A	115	ARG	HB3	1.64	0.022	2
1	A	115	ARG	CA	55.67	0.03	1
1	A	115	ARG	CB	29.96	0.03	1
1	A	115	ARG	CG	26.4	0.03	1
1	A	115	ARG	CD	42.78	0.03	1
1	A	115	ARG	N	119.97	0.04	1
1	A	116	GLU	H	8.37	0.022	1
1	A	116	GLU	HA	4.26	0.022	1
1	A	116	GLU	HB2	2.03	0.022	2
1	A	116	GLU	HB3	1.92	0.022	2
1	A	116	GLU	HG2	2.23	0.022	2
1	A	116	GLU	CA	55.89	0.03	1
1	A	116	GLU	CB	29.52	0.03	1
1	A	116	GLU	CG	35.64	0.03	1
1	A	116	GLU	N	121.85	0.04	1
1	A	117	SER	H	8.28	0.022	1
1	A	117	SER	HA	4.8	0.022	1
1	A	117	SER	HB2	3.79	0.022	2
1	A	117	SER	CA	57.62	0.03	1
1	A	117	SER	CB	63.02	0.03	1
1	A	117	SER	N	116.69	0.04	1
1	A	118	ILE	H	8.05	0.022	1
1	A	118	ILE	HA	4.18	0.022	1
1	A	118	ILE	HB	1.88	0.022	1
1	A	118	ILE	HG12	0.9	0.022	2
1	A	118	ILE	CA	60.64	0.03	1
1	A	118	ILE	CB	38.17	0.03	1
1	A	118	ILE	CG1	26.66	0.03	1
1	A	118	ILE	CG2	16.89	0.03	1
1	A	118	ILE	CD1	12.66	0.03	1
1	A	118	ILE	N	122.28	0.04	1
1	A	119	ASP	H	8.35	0.022	1
1	A	119	ASP	HA	4.61	0.022	1
1	A	119	ASP	HB2	2.74	0.022	1
1	A	119	ASP	HB3	2.58	0.022	1
1	A	119	ASP	CA	53.73	0.03	1
1	A	119	ASP	CB	40.55	0.03	1
1	A	119	ASP	N	123.84	0.04	1
1	A	120	MET	CA	55.19	0.03	1
1	A	120	MET	CB	31.68	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	MET	CG	28.25	0.03	1
1	A	120	MET	CE	19.53	0.03	1
1	A	121	GLY	H	8.49	0.022	1
1	A	121	GLY	HA2	4.5	0.022	2
1	A	121	GLY	C	173.95	0.03	1
1	A	121	GLY	CA	45.13	0.03	1
1	A	121	GLY	N	109.36	0.04	1
1	A	122	MET	H	8.11	0.022	1
1	A	122	MET	HA	4.24	0.022	1
1	A	122	MET	HB2	2.01	0.022	2
1	A	122	MET	HB3	1.86	0.022	2
1	A	122	MET	HG2	2.18	0.022	2
1	A	122	MET	C	175.05	0.03	1
1	A	122	MET	CA	54.85	0.03	1
1	A	122	MET	CB	29.31	0.03	1
1	A	122	MET	CG	31.42	0.03	1
1	A	122	MET	CE	19.75	0.03	1
1	A	122	MET	N	119.62	0.04	1
1	A	123	ASN	H	8.03	0.022	1
1	A	123	ASN	C	179.27	0.03	1
1	A	123	ASN	CA	54.34	0.03	1
1	A	123	ASN	CB	39.9	0.03	1
1	A	123	ASN	N	125.07	0.04	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	104	0.35 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	98	0.92 ± 0.14	Should be checked
$^{13}C'$	96	-0.09 ± 0.22	None needed (< 0.5 ppm)
^{15}N	99	0.19 ± 0.24	None needed (< 0.5 ppm)

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 70%, i.e. 945 atoms were assigned a chemical shift out of a possible 1348. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	419/510 (82%)	169/208 (81%)	168/202 (83%)	82/100 (82%)
Sidechain	526/775 (68%)	335/504 (66%)	184/246 (75%)	7/25 (28%)
Aromatic	0/63 (0%)	0/31 (0%)	0/26 (0%)	0/6 (0%)
Overall	945/1348 (70%)	504/743 (68%)	352/474 (74%)	89/131 (68%)

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: