wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1PMR
Title	:	LIPOYL DOMAIN FROM THE DIHYDROLIPOYL SUCCINYLTRANSFERASE COMPONENT OF THE 2-OXOGLUTARATE DEHYDROGENASE MULTIENZYME COMPLEX OF ESCHERICHIA COLI, NMR, 25 STRUCTURES
Authors	:	Ricaud, P.M.; Howard, M.J.; Roberts, E.L.; Broadhurst, R.W.; Perham, R.N.
Deposited on	:	1997-07-24

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:

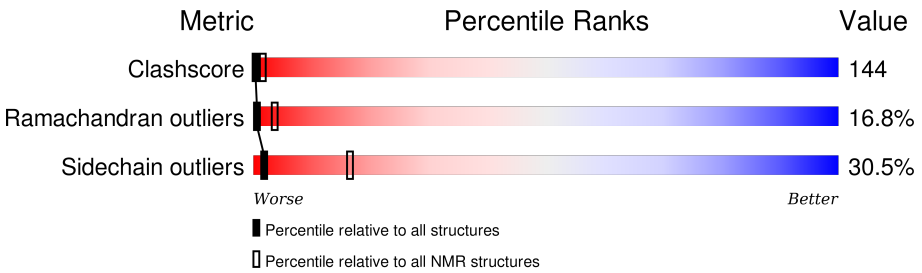
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal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

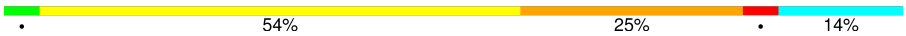
The overall completeness of chemical shifts assignment was not calculated.

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	80	

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 24 is the overall representative, medoid model (most similar to other models). The authors have identified model 21 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:2-A:9, A:17-A:77 (69)	0.35	24

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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1201 atoms, of which 602 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DIHYDROLIPOYL SUCCINYLTRANSFERASE.

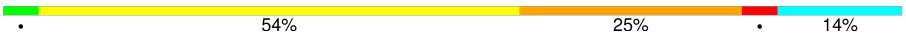
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	80	1201	371	602	100	128	0

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: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 

S1 S2 V3 D4 I5 L6 V7 P8 D9 L10 P11 E12 S13 V14 A15 D16 A17 T18 V19 A20 T21 W22 H23 K24 K25 P26 G27 D28 A29 V30 V31 R32 D33 E34 V35 L36 V37 E38 I39 E40 T41 D42 K43 V44 V45 L46 E47 V48 P49 A50 S51 A52 D53 G54 I55 L56 D57 A58 V59 L60

E61 D62 E63 G64 T65 T66 V67 T68 S69 R70 Q71 I72 L73 G74 R75 L76 R77 E78 G79 N80

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

The representative model is number 24. Colouring as in section 4.1 above.

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A:

S1 S2 V3 D4 I5 L6 V7 P8 D9 L10 P11 E12 S13 V14 A15 D16 A17 T18 V19 A20 T21 W22 H23 K24 K25 P26 G27 D28 A29 V30 V31 R32 D33 E34 V35 L36 V37 E38 I39 E40 T41 D42 K43 L46 E47 V48 P49 A50 S51 A52 D53 G54 I55 L56 D57 A58 V59 L60 E61

D62 E63 G64 T65 T66 V67 T68 S69 R70 Q71 I72 L73 G74 R75 L76 R77 E78 G79 N80

5 Refinement protocol and experimental data overview (i)

Of the 72 calculated structures, 25 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	refinement	3.1

No chemical shift data was provided. 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.

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	3.8±0.4
All	All	0	96

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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	75	ARG	Sidechain	25
1	A	32	ARG	Sidechain	24
1	A	70	ARG	Sidechain	24
1	A	77	ARG	Sidechain	23

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	521	533	533	152±8
All	All	13025	13325	13325	3807

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 144.

5 of 847 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:VAL:HG21	1:A:39:ILE:HD13	1.03	1.31	3	5
1:A:34:GLU:CG	1:A:50:ALA:HB3	1.03	1.84	13	9
1:A:37:VAL:HG21	1:A:73:LEU:HD21	1.01	1.33	14	5
1:A:56:LEU:HD12	1:A:76:LEU:CD1	1.01	1.84	22	3
1:A:3:VAL:HG12	1:A:5:ILE:CD1	1.00	1.84	6	2

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	69/80 (86%)	32±3 (46±4%)	26±3 (38±4%)	12±1 (17±2%)	0	3
All	All	1725/2000 (86%)	789 (46%)	647 (38%)	289 (17%)	0	3

5 of 25 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	37	VAL	25
1	A	28	ASP	25
1	A	33	ASP	25
1	A	52	ALA	24
1	A	55	ILE	20

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	59/68 (87%)	41±2 (69±4%)	18±2 (31±4%)	2	16
All	All	1475/1700 (87%)	1025 (69%)	450 (31%)	2	16

5 of 43 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	36	LEU	25
1	A	30	VAL	25
1	A	6	LEU	25
1	A	67	VAL	25
1	A	25	LYS	21

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)

No chemical shift data were provided