wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1FYC
Title	:	INNER LIPOYL DOMAIN FROM HUMAN PYRUVATE DEHYDROGENASE (PDH) COMPLEX, NMR, 1 STRUCTURE
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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:

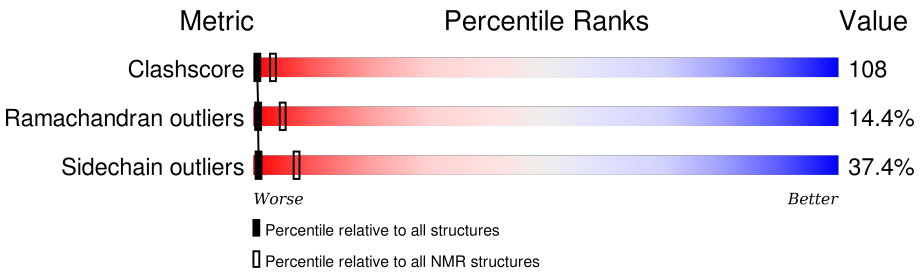
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 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	106	13% 56% 24% 8%

2 Ensemble composition and analysis (i)

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1639 atoms, of which 823 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DIHYDROLIPOAMIDE ACETYLTRANSFERASE (E2P).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	106	1639	518	823	129	164	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASN	-	INSERTION	UNP P10515
A	4	MET	-	INSERTION	UNP P10515

4 Residue-property plots (i)

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: DIHYDROLIPOAMIDE ACETYLTRANSFERASE (E2P)

Chain A: 13% 56% 24% 8%

G1 S2 N3 M4 S5 Y6 P7 P8 H9 M10 Q11 V12 L13 L14 P15 A16 L17 S18 P19 T20 M21 T22 M23 G24 T25 V26 Q27 R28 W29 E30 K31 K32 V33 G34 E35 K36 L37 S38 E39 G40 D41 L42 L43 A44 E45 I46 E47 T48 D49 K50 A51 T52 I53 G54 F55 E56 V57 Q58 E59 E60

G61 Y62 L63 A64 K65 I66 L67 V68 P69 E70 G71 T72 R73 D74 V75 P76 L77 G78 T79 P80 L81 C82 I83 I84 V85 E86 K87 E88 A89 D90 I91 S92 A93 F94 R98 P99 T100 E101 D104 L105 K106

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 80 calculated structures, 1 were deposited, based on the following criterion: *MEAN STRUCTURE FROM 26 CHOSEN HAVING LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
ANSIG	structure solution	3.3

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	3
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	28	ARG	Sidechain
1	A	98	ARG	Sidechain
1	A	73	ARG	Sidechain

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	816	823	823	177
All	All	816	823	823	177

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 108.

5 of 177 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:12:VAL:HG12	1:A:82:CYS:C	0.89	1.87

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:65:LYS:CB	1:A:83:ILE:HG22	0.87	1.99
1:A:65:LYS:HB3	1:A:83:ILE:HG22	0.85	1.49
1:A:12:VAL:O	1:A:81:LEU:HD23	0.84	1.72
1:A:74:ASP:O	1:A:75:VAL:HG13	0.82	1.74

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	104/106 (98%)	53 (51%)	36 (35%)	15 (14%)	1 5
All	All	104/106 (98%)	53 (51%)	36 (35%)	15 (14%)	1 5

5 of 15 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	60	GLU
1	A	6	TYR
1	A	85	VAL
1	A	33	VAL
1	A	2	SER

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	91/91 (100%)	57 (63%)	34 (37%)	1 7
All	All	91/91 (100%)	57 (63%)	34 (37%)	1 7

5 of 34 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	52	THR
1	A	101	GLU
1	A	10	MET
1	A	70	GLU
1	A	83	ILE

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