

Structural architecture of NDE1 and NDEL1 in solution

Protein	Oligomeric state	AA1	AA2	Minimum Ca to Ca distance in Å (2V71; aa8–167)	Minimum Ca to Ca distance in Å (2V66; aa58–168)	Replication status or equivalent residues in cross-linked contact
NDEL1	Dimer	K20	K27	10.43 (intra)	n/a	In NDEL1 tetramer
NDEL1	Dimer	K25	K27	5.43 (intra)	n/a	In NDEL1 tetramer
NDEL1	Dimer	K27	K27	7.78 (inter)	n/a	
NDEL1	Dimer	K80	K82	5.54 (intra)	n/a	In NDEL1 tetramer, NDE1 dimer, NDE1 tetramer
NDEL1	Dimer	S90	S95	8.21 (intra)	n/a	
NDEL1	Dimer	K108	K108	13.92 (inter)	n/a	In NDEL1 tetramer, NDE1 dimer, NDE1 tetramer
NDEL1	Dimer	K108	Y114	9.77 (intra)	n/a	
NDEL1	Tetramer	K20	K27	10.43 (intra)	n/a	In NDEL1 dimer
NDEL1	Tetramer	K25	K27	5.43 (intra)	n/a	In NDEL1 dimer
NDEL1	Tetramer	K27	S29	5.48 (intra)	n/a	
NDEL1	Tetramer	K80	K82	5.54 (intra)	5.35 (intra)	In NDEL1 dimer, NDE1 dimer, NDE1 tetramer
NDEL1	Tetramer	K80	S90	15.15 (intra)	15.15 (intra)	
NDEL1	Tetramer	K108	K108	13.92 (inter)	12.91 (inter)	In NDEL1 dimer, NDE1 dimer, NDE1 tetramer
NDEL1	Tetramer	K108	K113	8.86 (intra)	8.62 (intra)	In NDE1 tetramer
				Minimum Ca to Ca distance in Å (homology model; aa7–166)	Minimum Ca to Ca distance in Å (homology model; aa57–167)	
NDE1	Dimer	K79	K81	5.36 (intra)	n/a	In NDEL1 dimer, NDEL1 tetramer
NDE1	Dimer	K81	S94	20.01 (intra)	n/a	
NDE1	Dimer	K107	K107	13.91 (inter)	n/a	In NDEL1 dimer, NDEL1 tetramer
NDE1	Tetramer	K79	K81	5.36 (intra)	5.30 (intra)	In NDE1 dimer, NDEL1 dimer, NDEL1 tetramer
NDE1	Tetramer	K81	K107	36.17 (inter)	36.15 (inter)	
NDE1	Tetramer	K107	K107	13.91 (inter)	12.90 (inter)	In NDE1 dimer, NDEL1 dimer, NDEL1 tetramer
NDE1	Tetramer	K107	K112	8.76 (intra)	8.57 (intra)	In NDEL1 tetramer
				Minimum Ca to Ca distance in Å (homology model; aa7–166, 8-167)	Minimum Ca to Ca distance in Å (homology model; aa57–167, 58-168)	
NDE1-NDEL1	Tetramer	K107 (NDE1)	K108 (NDEL1)	69.38 (inter protein)	68.03 (inter protein)	While this contact is between two different proteins, the equivalent residues were seen in the pure NDEL1 dimer, NDEL1 tetramer,

						NDE1 dimer and NDE1 tetramer
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SUPPLEMENTAL TABLE 3: Mapping cross-linking data on the crystal structures of NDEL1 and homology models of NDE1 and NDE1-NDEL1.

Only cross-links that reside entirely within the region of the solved crystal structures (PDB IDs: 2V71 and 2V66) and the equivalent homology models of NDE1 and NDE1-NDEL1 are shown. Amino acids 8-167 were solved in the 2V71 crystal structure, while the shorter 2V66 structure contains amino acids 58-168. The 2V71 NDEL1 8-167 structure was deposited as a dimer in the PDB and a tetramer was generated as described previously using symmetry operations. The 2V66 NDEL1 58-168 structure was deposited as a tetramer. If a cross-link resided in a dimer, then each dimer was independently analyzed and all possible combinations of distances measured; only the lowest distance occurrence, either inter-chain or intra-chain is shown in the Table. In each case the oligomeric state, the specific amino acid residues involved (AA1 and AA2) in the cross-link peptides is provided. If a cross-link was noted in another oligomeric state or experiment, these are indicated in the 'Replication status' column. The distances were measured between the alpha Carbon atoms for a cross-linked pair of residues. Where self-residue cross-links occur, these are colored green indicating inter-chain contacts. The closest cross-link pairs seen in the NDEL1 dimer and tetramer, in the NDE1 dimer and tetramer, and in the NDE-NDEL1 tetramer that can be mapped on the longer crystal structure fragment (2V71) and the homology models are shown in Fig. 5 and 6 in the main text. Note, in some cases more than one mapped distance between residues is sufficiently close at the level of alpha Carbon atoms ($< 27 \text{ \AA}$) to form feasible cross-links, but in this table only the closest cross-linked pair distances are provided for either the intra- or inter-chain linkage.